The Fermilab HEPCloud, or How to add 240 TFlops in an hour or two*

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Middleware and Grid Interagency Coordination (MAGIC) / NITRD

January 4, 2017

* Or three. Four at the most.

Disclaimer

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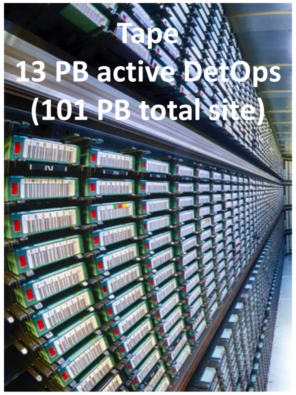
Changing Roles of HEP Facilities

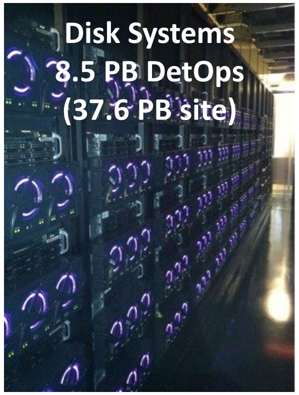
- Strategic Plan for U.S. Particle Physics (P5 Report)

  Rapidly evolving computer architectures and increasing data volumes require effective crosscutting solutions that are being developed in other science disciplines and in industry. Mechanisms are needed for the continued maintenance and development of major software frameworks and tools for particle physics and long-term data and software preservation, as well as investments to exploit next-generation hardware and computing models.

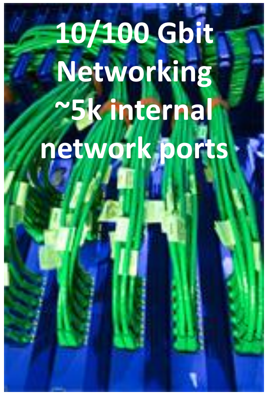
HTC, HPC Cores
15.5K DetOps
23K CMS
(68.7K total site)



Tape
13 PB active DetOps
(101 PB total site)



Disk Systems
8.5 PB DetOps
(37.6 PB site)

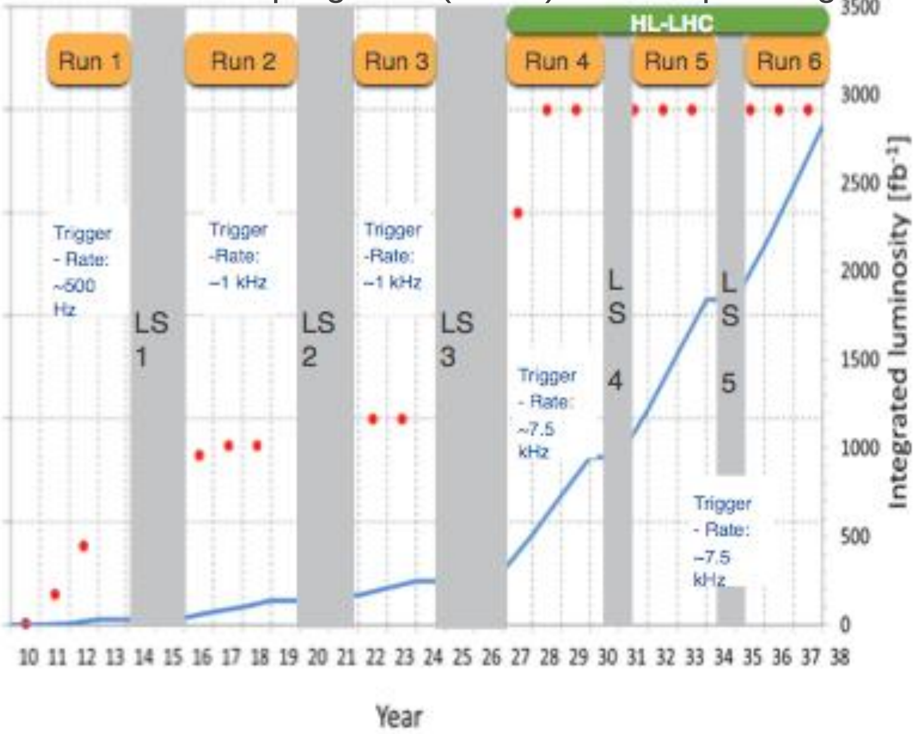


10/100 Gbit
Networking
~5k internal
network ports

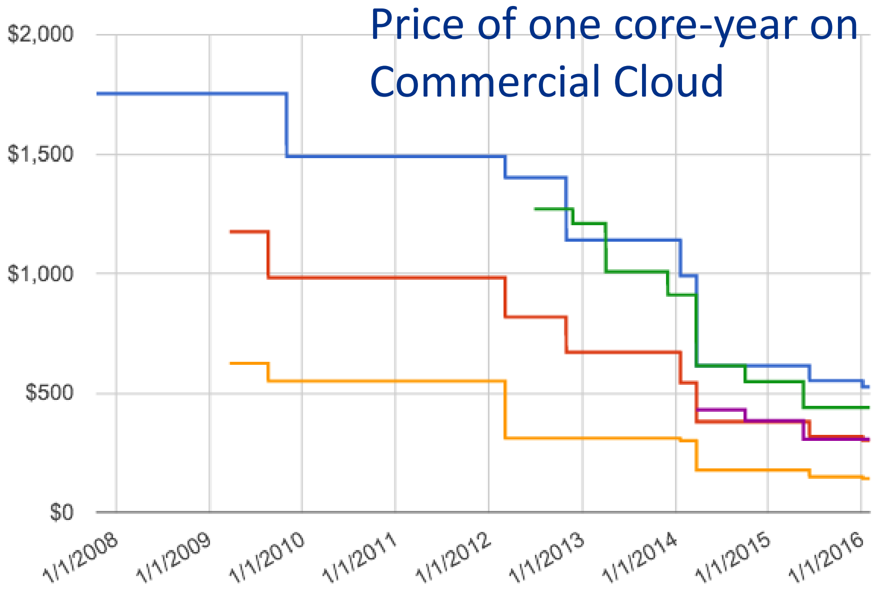
- Need to evolve the facility beyond present infrastructure

Drivers for Evolving the Facility: Capacity and Cost

- High Energy Physics computing needs will be 10-100x current capacity
  - Two new programs coming online (DUNE, High-Luminosity LHC), while new physics search programs (Mu2e) will be operating

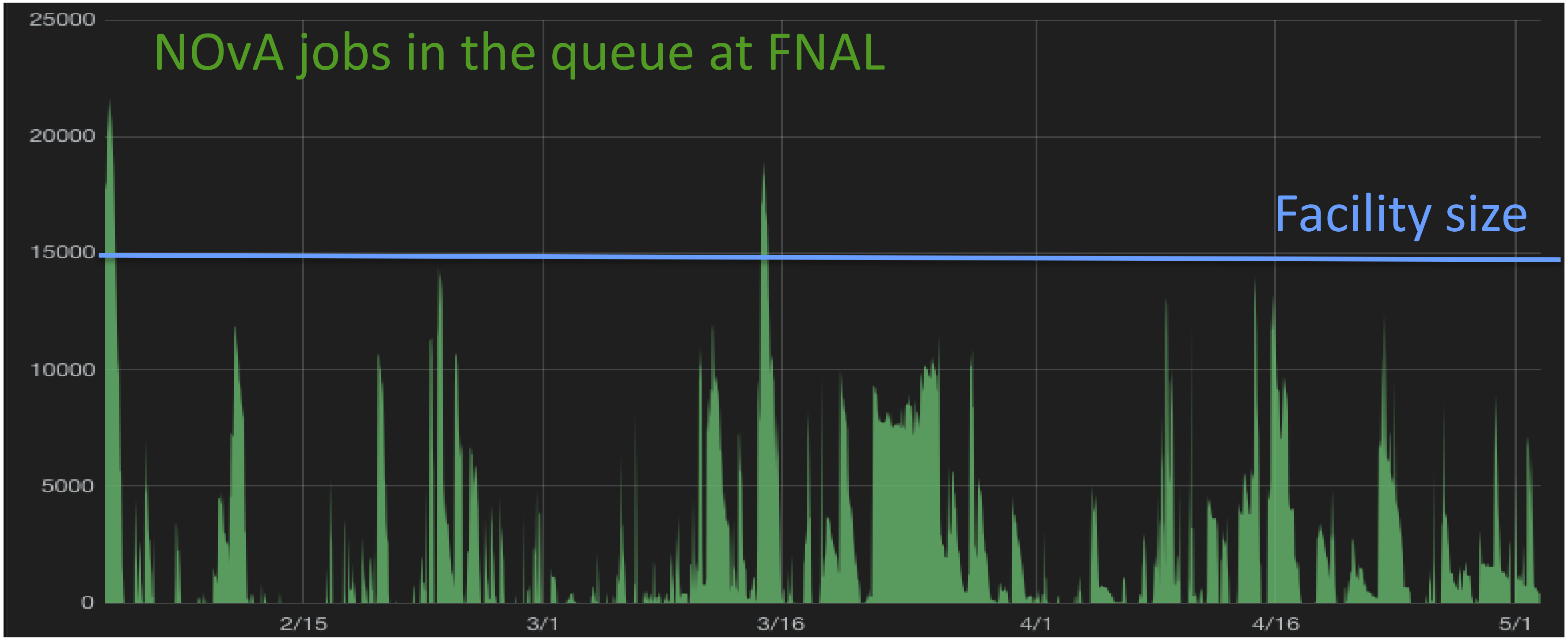


- Scale of industry at or above R&D
  - Commercial clouds offering increased **value** for decreased **cost** compared to the past


Price of one core-year on Commercial Cloud

Drivers for Evolving the Facility: Elasticity

- Usage is not steady-state
- Computing schedules driven by real-world considerations (detector, accelerator, …) but also ingenuity – this is research and development of cutting-edge science



Classes of Resource Providers

Grid

- Virtual Organizations (VOs) of users trusted by Grid sites
- VOs get allocations ➜ **Pledges**
  - Unused allocations: opportunistic resources

“Things you borrow”

Trust Federation

Cloud

- Community Clouds - Similar trust federation to Grids
- Commercial Clouds - **Pay-As-You-Go** model
  - Strongly accounted
  - Near-infinite capacity ➜ **Elasticity**
  - Spot price market

“Things you rent”

Economic Model

HPC

- Researchers granted access to HPC installations
- Peer review committees award **Allocations**
  - Awards model designed for individual PIs rather than large collaborations

“Things you are given”

Grant Allocation

HEPCloud: the Evolved Facility

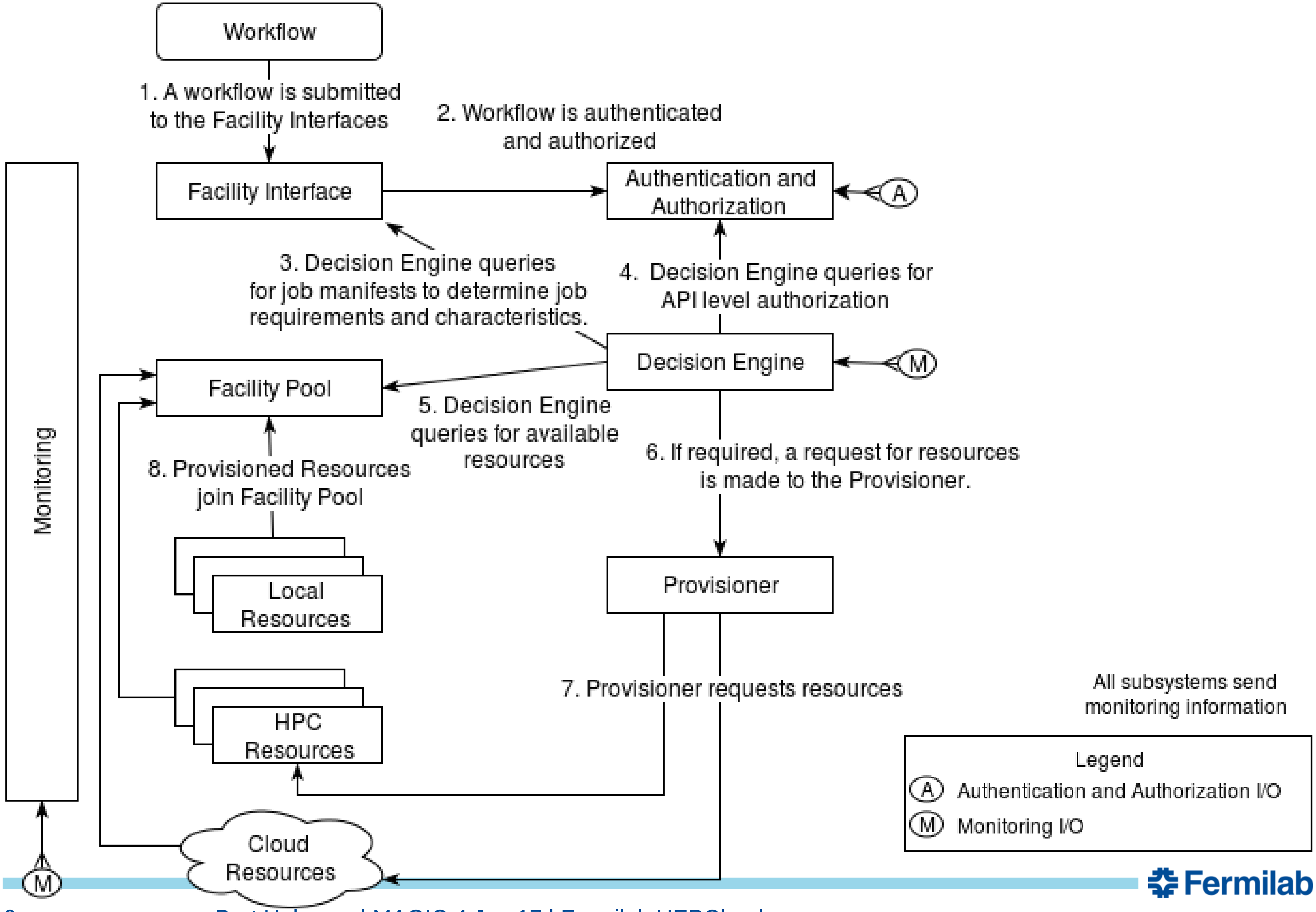
- Vision Statement
  - HEPCloud is envisioned as a portal to an ecosystem of diverse computing resources commercial or academic
  - Provides “complete solutions” to users, with agreed upon levels of service
  - The Facility routes to local or remote resources based on workflow requirements, cost, and efficiency of accessing various resources
  - Manages allocations of users to target compute engines
- Pilot project to explore feasibility, capability of HEPCloud
  - Goal of moving into production during FY18
  - Seed money provided by industry

HEPCloud Collaborations

- Participate in collaboration to leverage tools and experience whenever possible

- Grid technologies – Worldwide LHC Computing Grid
  - Preparing communities for distributed computing
- BNL and ATLAS, ANL – engaged in next HEPCloud phase
- HTCondor – common provisioning interface
- CMS, IF experiments – collaborative knowledge and tools, cloud-capable workflows
- CERN faces similar challenges and we are having productive conversations with different facets
  - For example - CERN openlab CTO is engaged in HEPCloud

HEPCloud Architecture



Workflow

1. A workflow is submitted to the Facility Interfaces

Facility Interface

2. Workflow is authenticated and authorized

Authentication and Authorization

A

3. Decision Engine queries for job manifests to determine job requirements and characteristics.

4. Decision Engine queries for API level authorization

Decision Engine

M

Facility Pool

5. Decision Engine queries for available resources

6. If required, a request for resources is made to the Provisioner.

8. Provisioned Resources join Facility Pool

Local Resources

Provisioner

Monitoring

HPC Resources

7. Provisioner requests resources

All subsystems send monitoring information

Legend

A Authentication and Authorization I/O

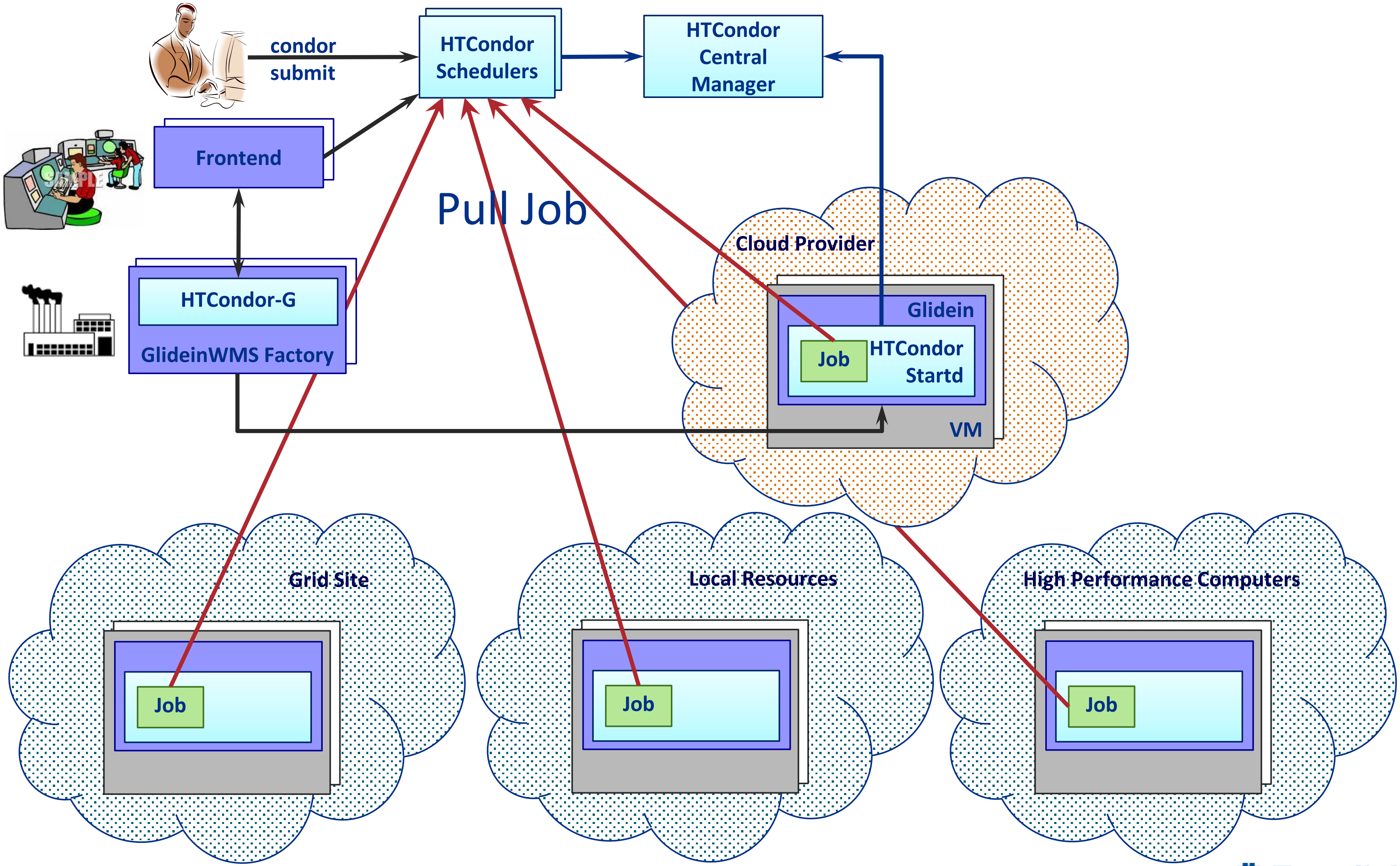
M Monitoring I/O

Cloud Resources

M

Fermilab

HEPCloud – glideinWMS and HTCondor



Early 2016 HEPCloud Use Cases - AWS

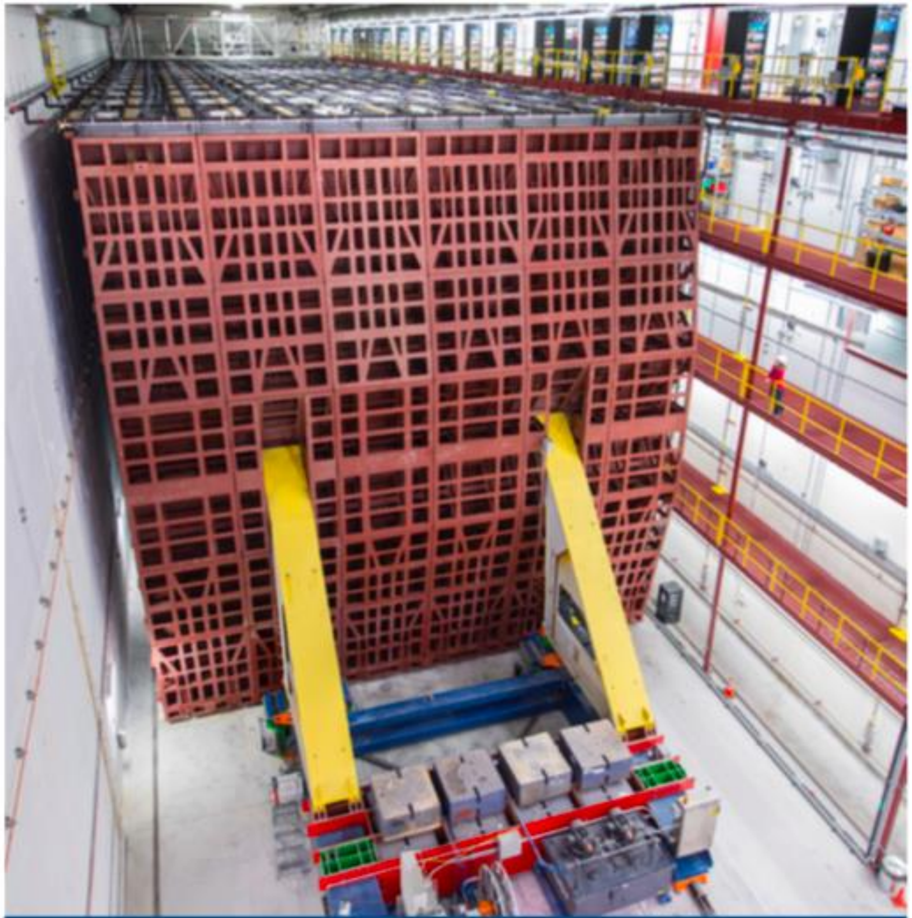
NoVA Processing

Processing the 2014/2015 dataset
16 4-day "campaigns" over one year
Demonstrates stability, availability, cost-effectiveness
Received AWS academic grant

CMS Monte Carlo Simulation

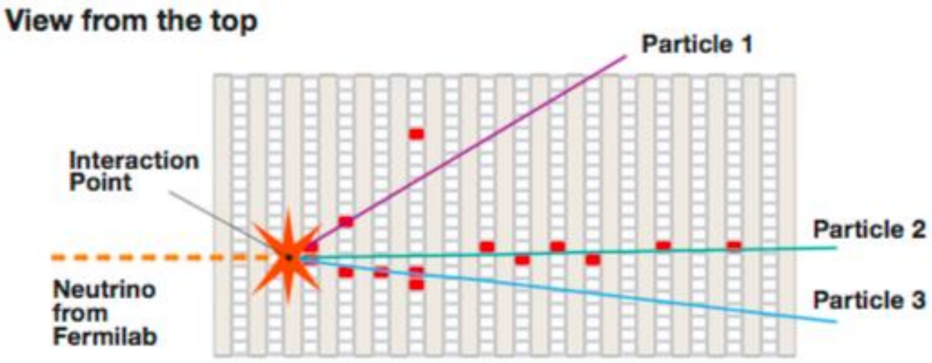
Generation (and detector simulation, digitization, reconstruction) of simulated events in time for Moriond16 conference
56000 compute cores, steady-state
Demonstrates scalability
Received AWS academic grant

NOvA: Neutrino Experiment



The NOvA detector in Minnesota occupies an area about the size of two basketball courts. It is 200 feet long and made of modules 50 feet high and 50 feet wide. The detector records particle tracks from neutrinos sent by a powerful accelerator at Fermilab. The construction of the NOvA detectors was completed in the fall of 2014, on time and under budget. The experiment is scheduled to collect information for six years.

Neutrino interaction recorded by NOvA



Neutrinos rarely interact with matter. When a neutrino smashes into an atom in the NOvA detector in Minnesota, it creates distinctive particle tracks. Scientists explore these particle interactions to better understand the transition of muon neutrinos into electron neutrinos. The experiment also helps answer important scientific questions about neutrino masses, neutrino oscillations, and the role neutrinos played in the early universe.

NOvA Use Case

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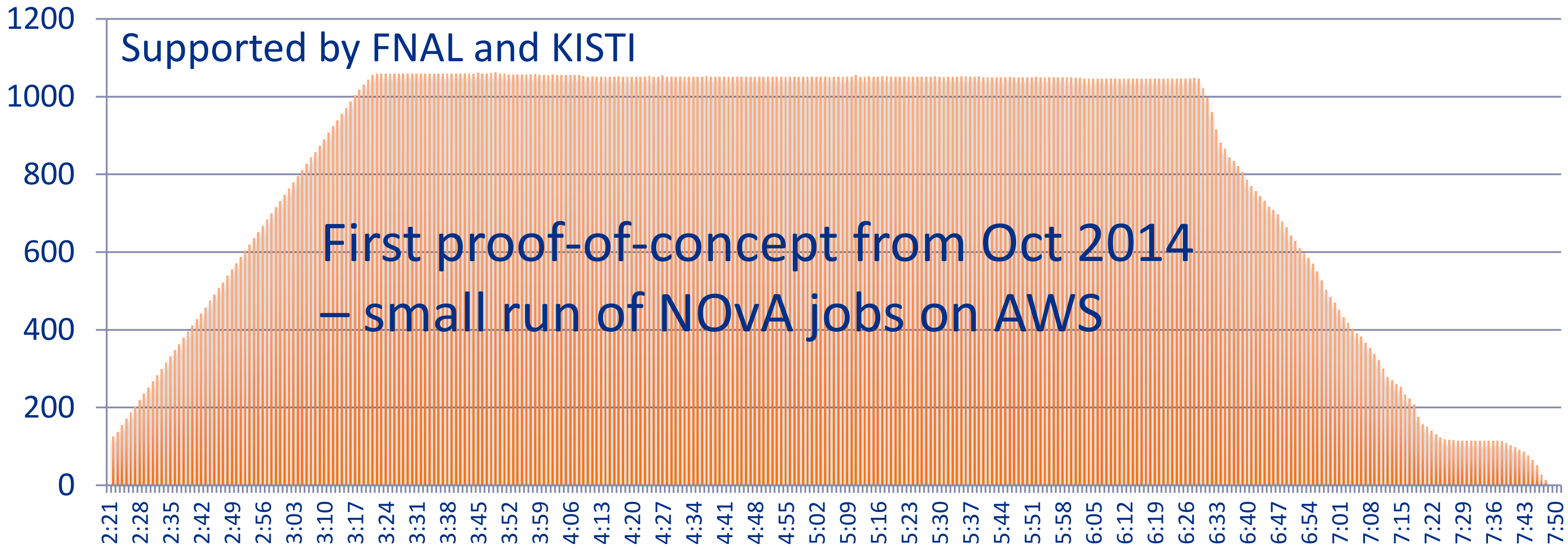
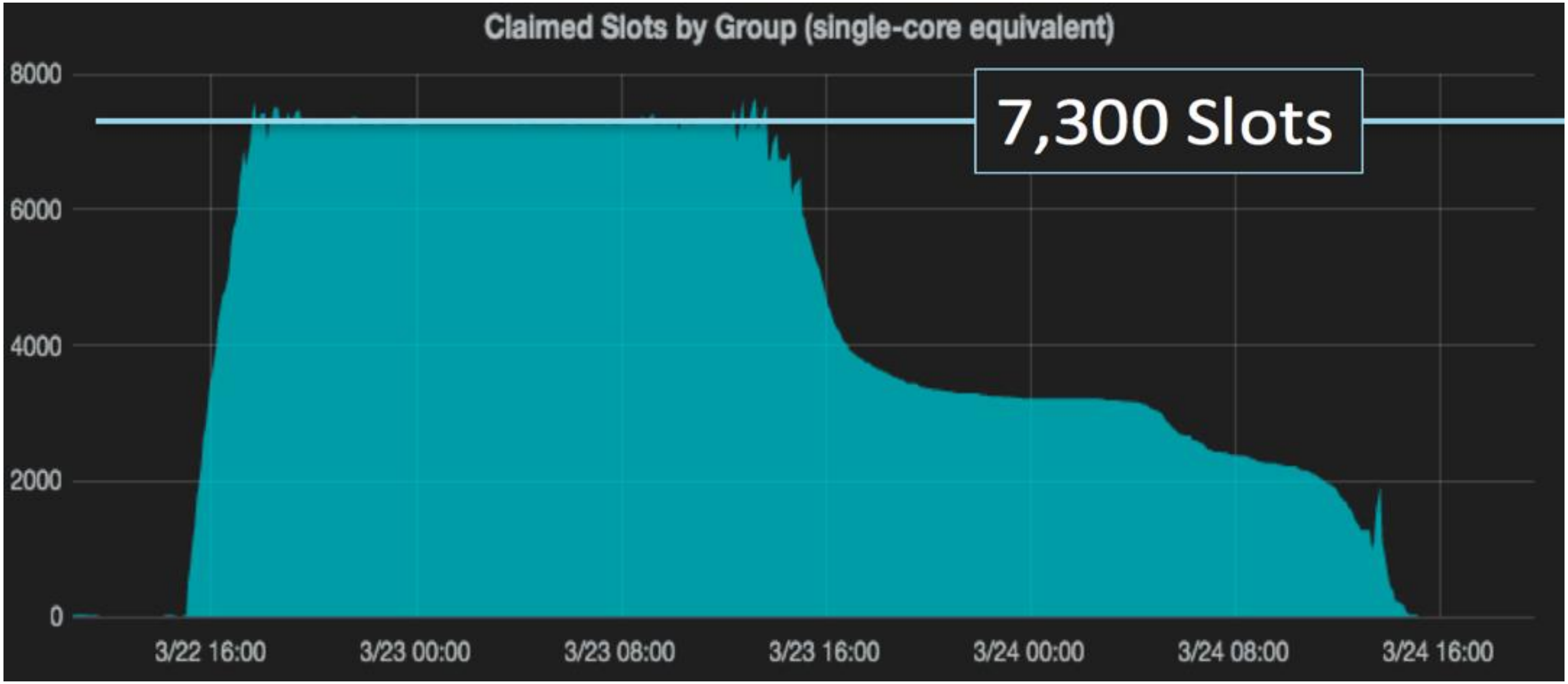


Supported by FNAL and KISTI

First proof-of-concept from Oct 2014 – small run of NOvA jobs on AWS

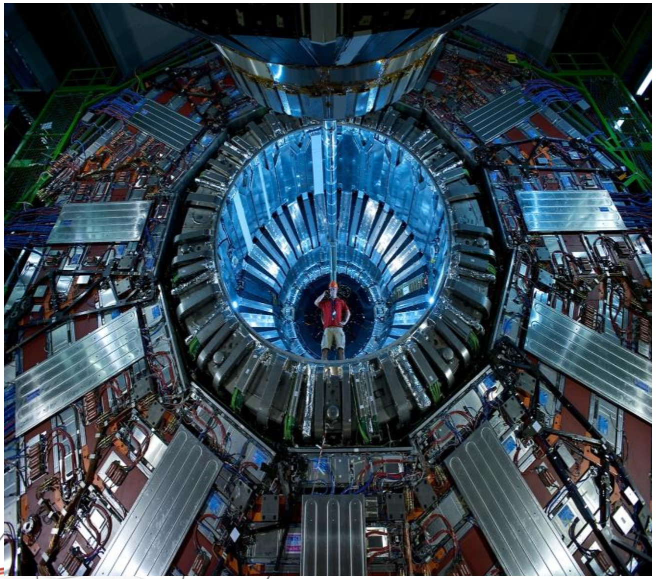
NOvA Use Case – running at 7300 cores

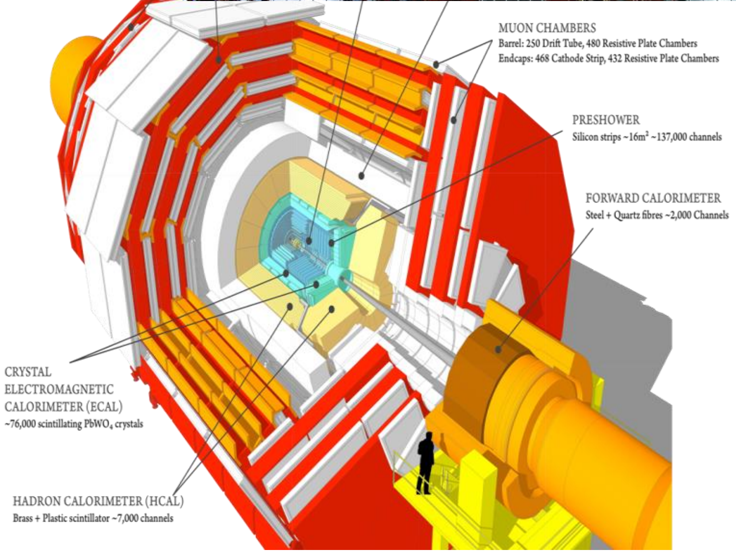
- Added support for general-purpose data-handling tools (SAM, IFDH, F-FTS) for AWS Storage and used them to stage both input datasets and job outputs



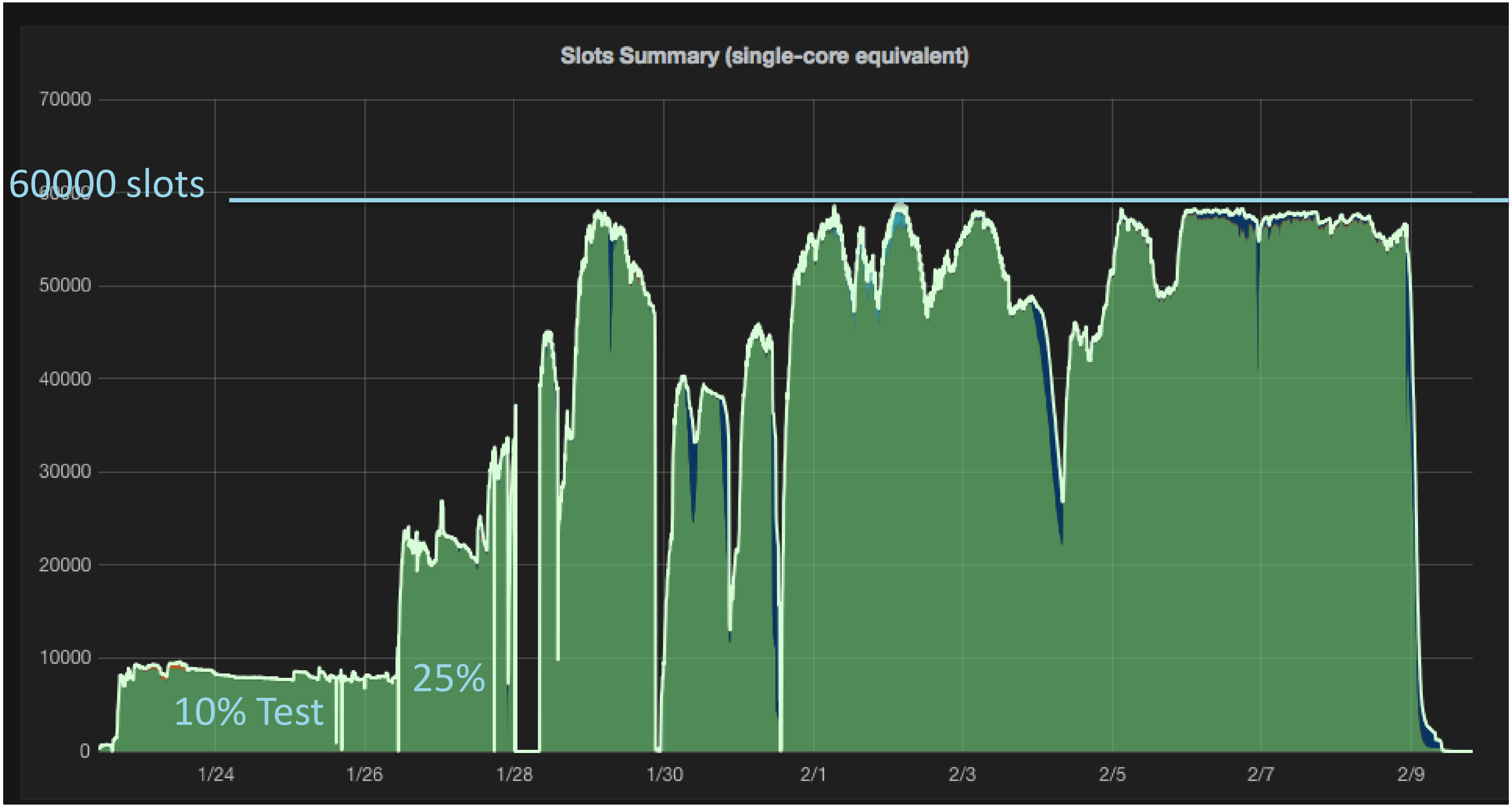
Compact Muon Solenoid (CMS)

- Detector built around collision point
  - One of four detectors at the Large Hadron Collider
- Records flight path and energy of all particles produced in a collision
- 100 Million individual measurements (channels)
- All measurements of a collision together are called: **event**
- **We need to simulate many billions of events**

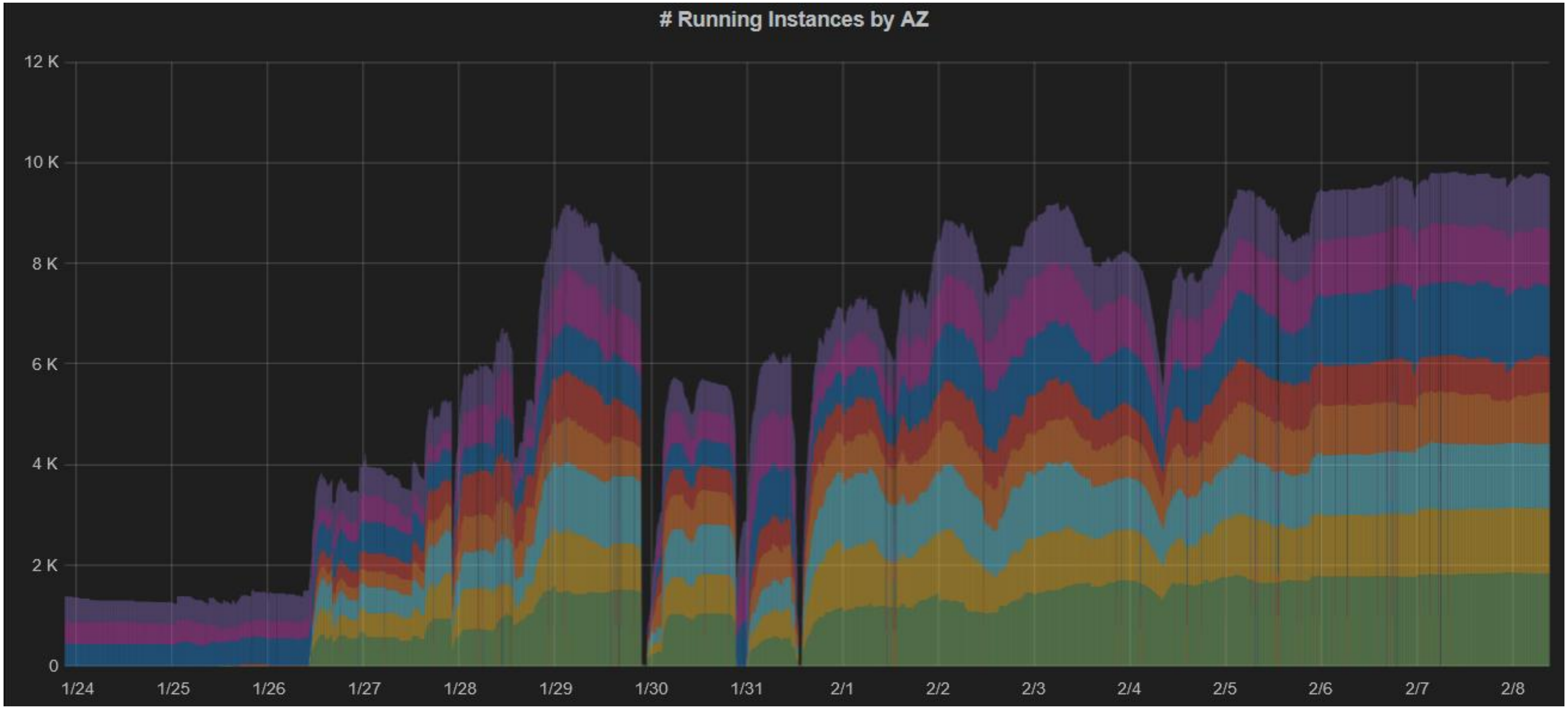



CMS DETECTOR
Total weight : 14,000 tonnes
Overall diameter : 15.0 m
Overall length : 28.7 m
Magnetic field : 3.8 T
MUON CHAMBERS
Barrel: 250 Drift Tube, 480 Resistive Plate Chambers
Endcaps: 468 Cathode Strip, 432 Resistive Plate Chambers
PRESHOWER
Silicon strips ~16m² ~137,000 channels
FORWARD CALORIMETER
Steel + Quartz fibres ~2,000 Channels
CRYSTAL ELECTROMAGNETIC CALORIMETER (ECAL)
~76,000 scintillating PbWO₄ crystals
HADRON CALORIMETER (HCAL)
Brass + Plastic scintillator ~7,000 channels

Reaching ~60k slots on AWS with FNAL HEPCloud

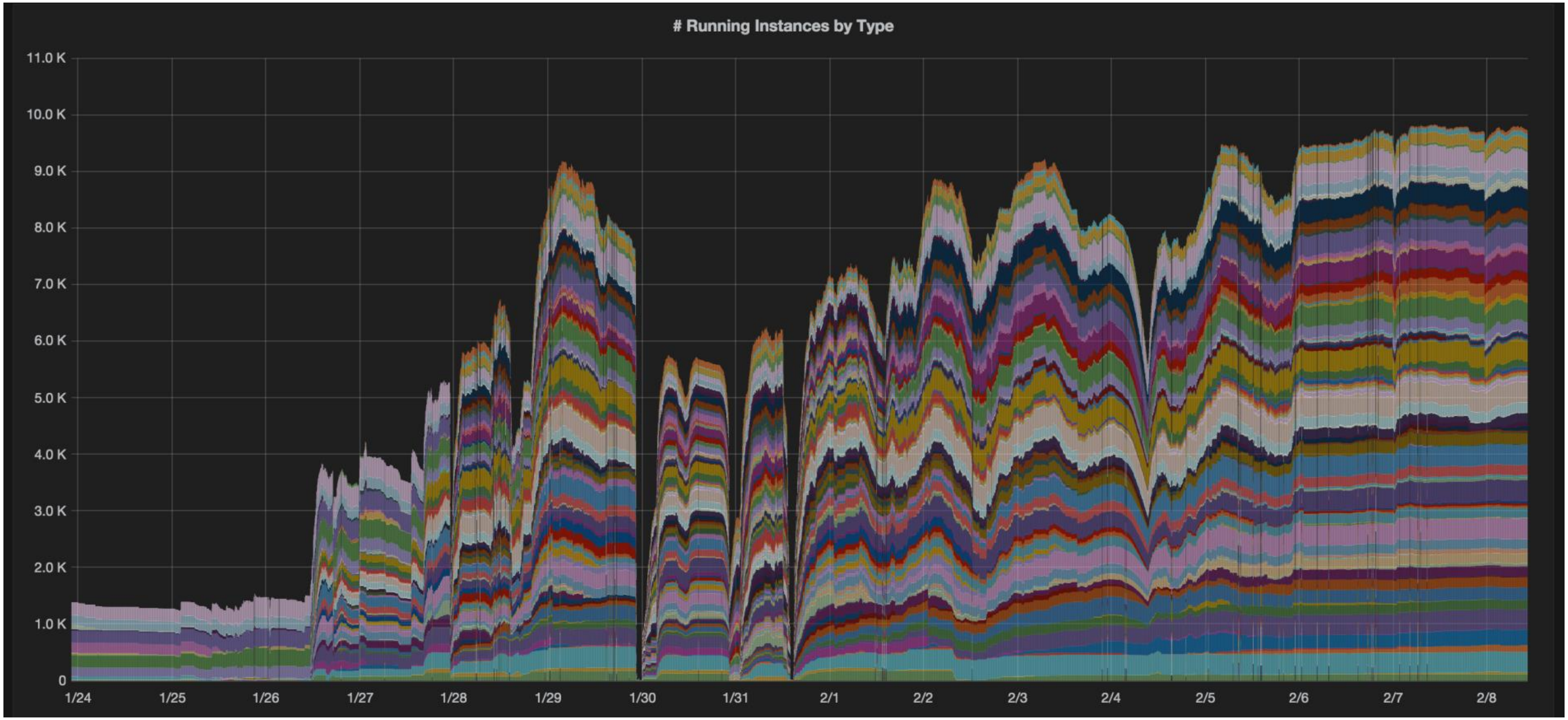


HEPCloud AWS slots by Region/Zone



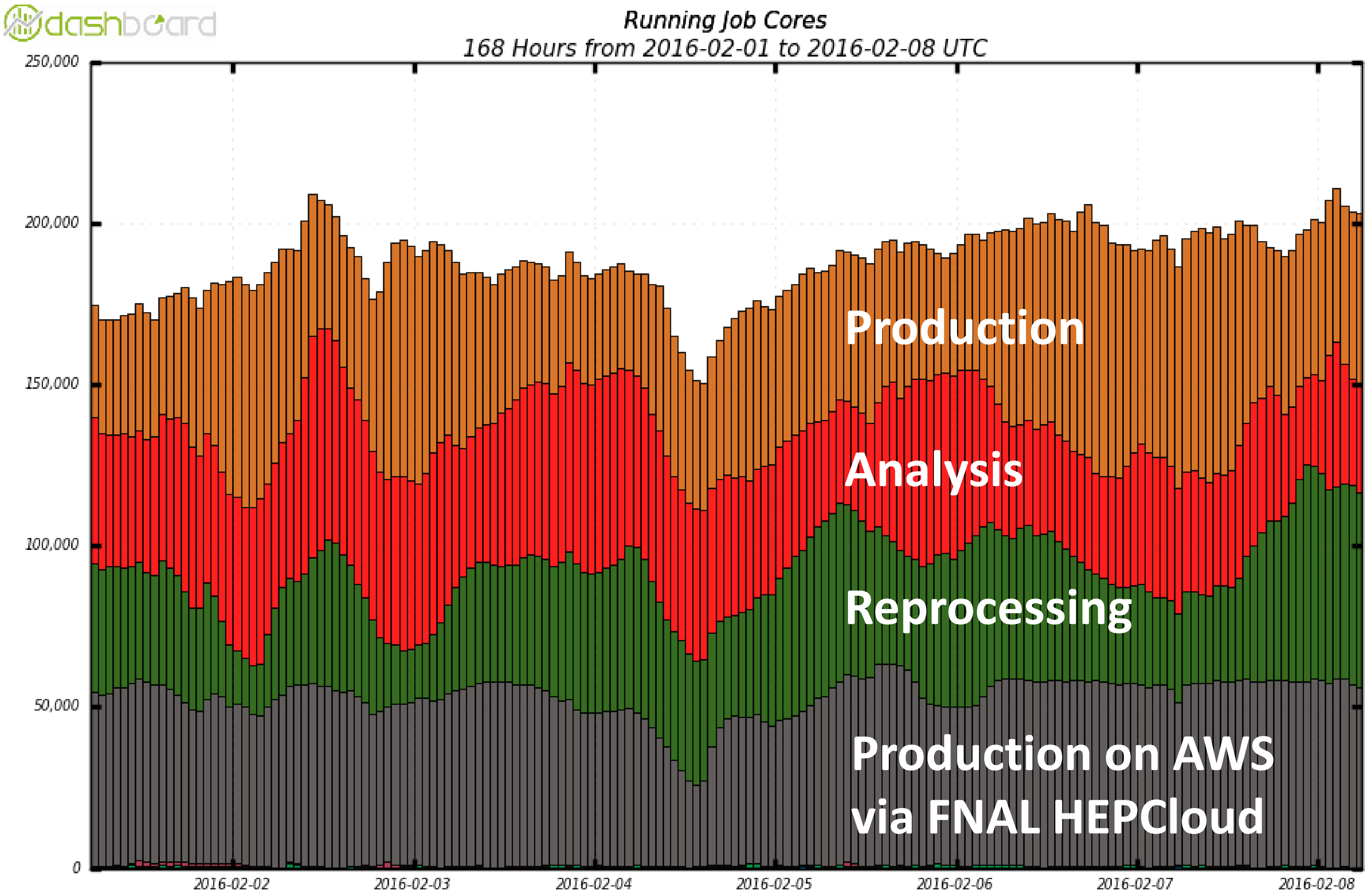
Each color corresponds to a different region+zone

HEPCloud AWS slots by Region/Zone/Type

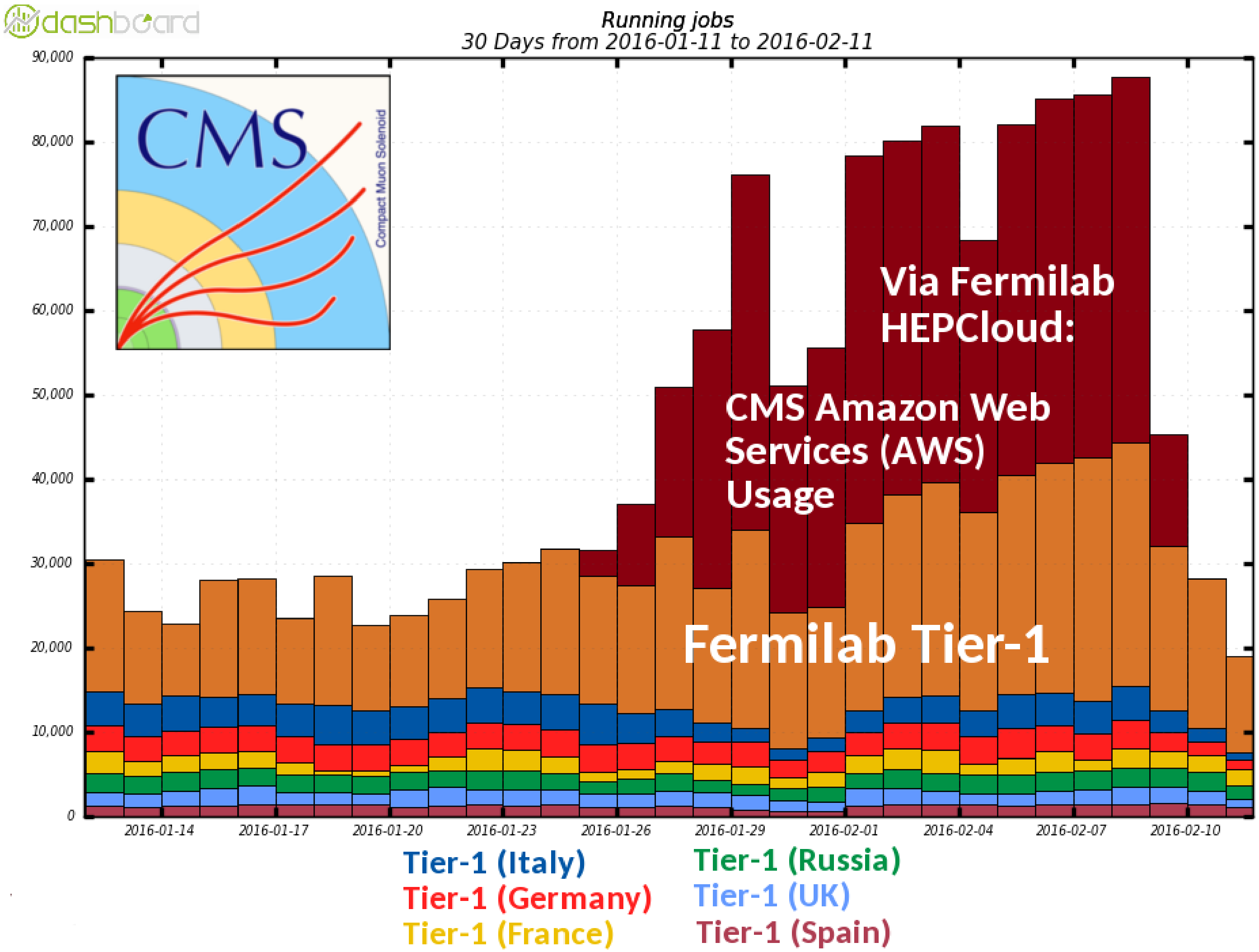


Each color corresponds to a different region+zone+machine type

HEPCloud AWS: 25% of CMS global capacity

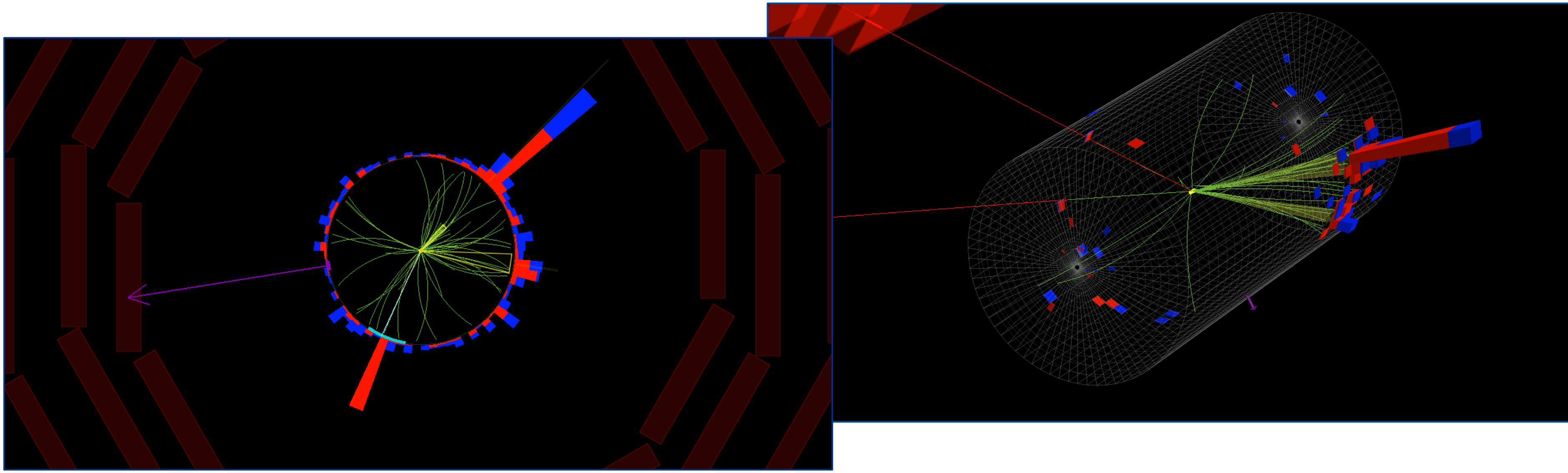


Fermilab HEPCloud compared to global CMS Tier-1



Results from the Jan 2016 CMS Use Case

- **All CMS simulation requests fulfilled for conference**
  - **2.9 million jobs, 15.1 million wall hours**
    - 9.5% badput – including preemption
    - 87% CPU efficiency
  - **518 million events generated**



Late 2016 HEPCloud Use Cases - Google

NoVA Processing

Processing the 2014/2015 dataset
16 4-day “campaigns” over one year
Demonstrates stability, availability, cost-effectiveness
Received AWS academic grant

CMS Monte Carlo Simulation

Generation (and detector simulation, digitization, reconstruction) of simulated events in time for Moriond16 conference
56000 compute cores, steady-state
Demonstrates scalability
Received AWS academic grant

CMS Monte Carlo Simulation

Generation (and detector simulation, digitization, reconstruction) of simulated events in time for Moriond17 conference
160000 compute cores during Supercomputing 2016 conference (~48 h)
Demonstrates scalability, capability
Received Google Cloud Platform grant

mu2e Processing

Simulating cosmic ray veto detector and beam particle backgrounds
3M integrated core-hours
Demonstrates rapid on-boarding
Received Google Cloud Platform grant

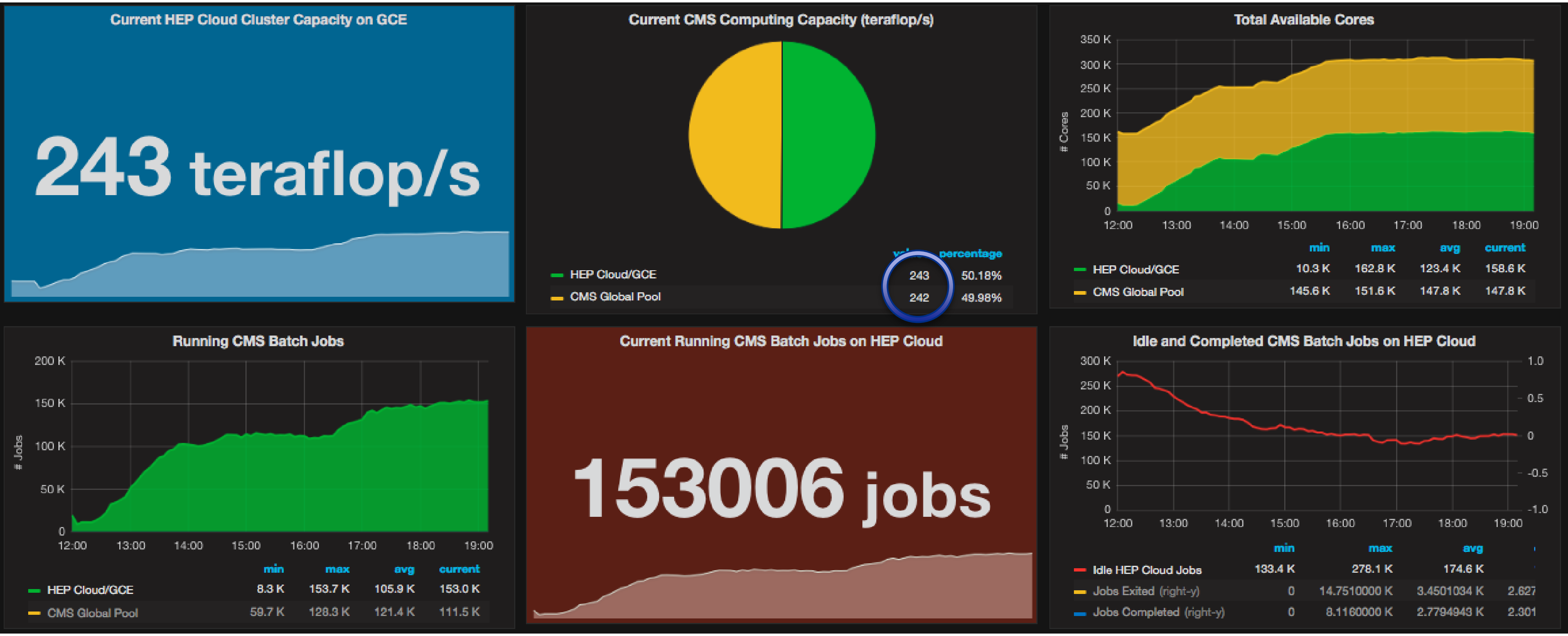
Results from the Jan 2016 CMS Use Case

- **All CMS simulation requests fulfilled for conference**
  - **2.9 million jobs, 15.1 million wall hours**
    - 9.5% badput – including preemption
    - 87% CPU efficiency
  - **518 million events generated**

- **Supercomputing 2016**
  - **Aiming to generate* 1 Billion events in 48 hours during Supercomputing 2016**
  - **Double the size of global CMS computing resources**

* 35% filter efficiency – 380 million events staged out

https://fifemon.fnal.gov/hcf/dashboard/db/hep-cloud-demo?from=now-12h&to=1479172229000

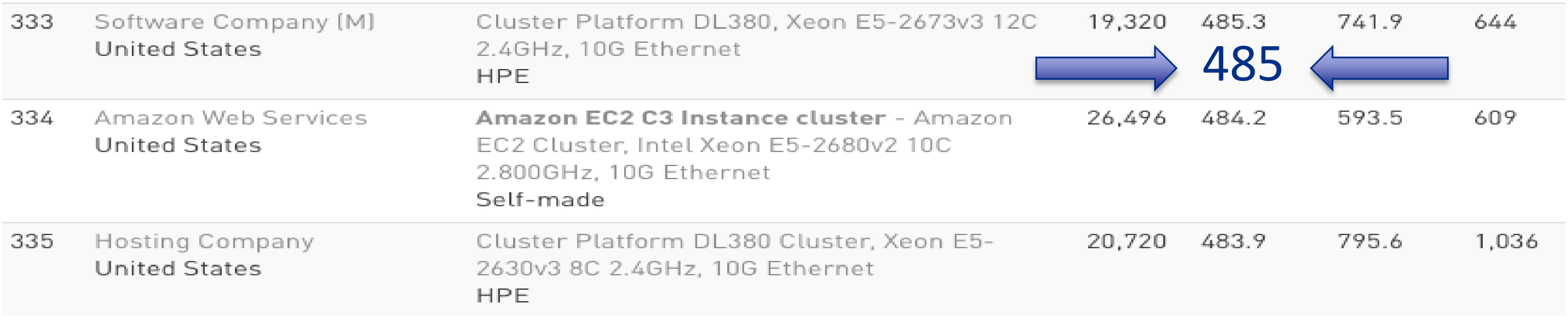


	value	percentage
🟩 HEP Cloud/GCE	243	50.18%
🟨 CMS Global Pool	242	49.98%

	min	max	avg	current
🟩 HEP Cloud/GCE	10.3 K	162.8 K	123.4 K	158.6 K
🟨 CMS Global Pool	145.6 K	151.6 K	147.8 K	147.8 K

	min	max	avg	current
🟩 HEP Cloud/GCE	8.3 K	153.7 K	105.9 K	153.0 K
🟨 CMS Global Pool	59.7 K	128.3 K	121.4 K	111.5 K

	min	max	avg	
🟥 Idle HEP Cloud Jobs	133.4 K	278.1 K	174.6 K	
🟨 Jobs Exited (right-y)	0	14.7510000 K	3.4501034 K	2.627
🟦 Jobs Completed (right-y)	0	8.1160000 K	2.7794943 K	2.301



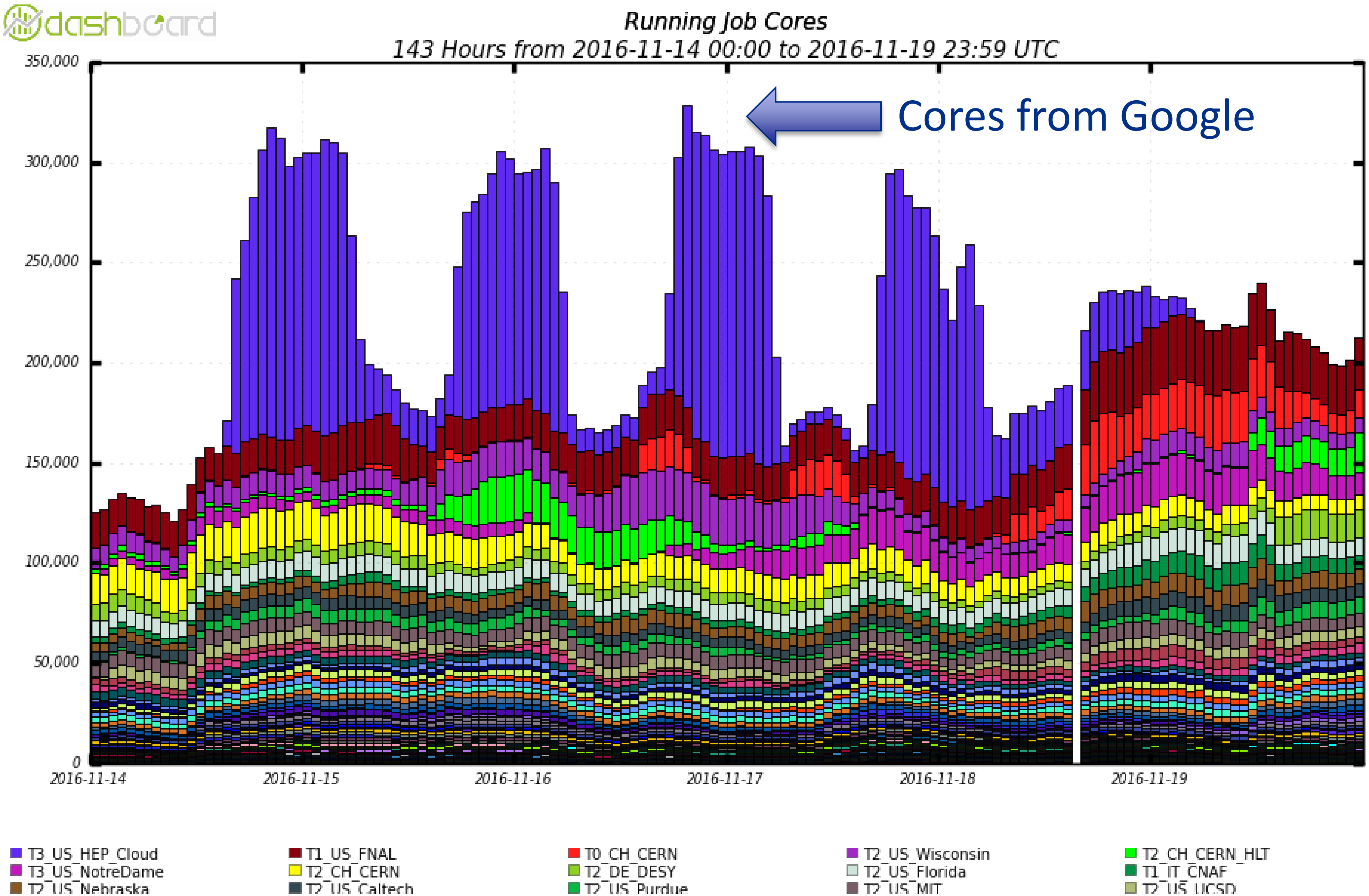
333	Software Company (M) United States	Cluster Platform DL380, Xeon E5-2673v3 12C 2.4GHz, 10G Ethernet HPE	19,320	485.3	741.9	644
334	Amazon Web Services United States	**Amazon EC2 C3 Instance cluster** - Amazon EC2 Cluster, Intel Xeon E5-2680v2 10C 2.800GHz, 10G Ethernet Self-made	26,496	484.2	593.5	609
335	Hosting Company United States	Cluster Platform DL380 Cluster, Xeon E5-2630v3 8C 2.4GHz, 10G Ethernet HPE	20,720	483.9	795.6	1,036

→ 485 ←

334 on the Top500 list?

Fermilab

Doubling CMS compute capacity

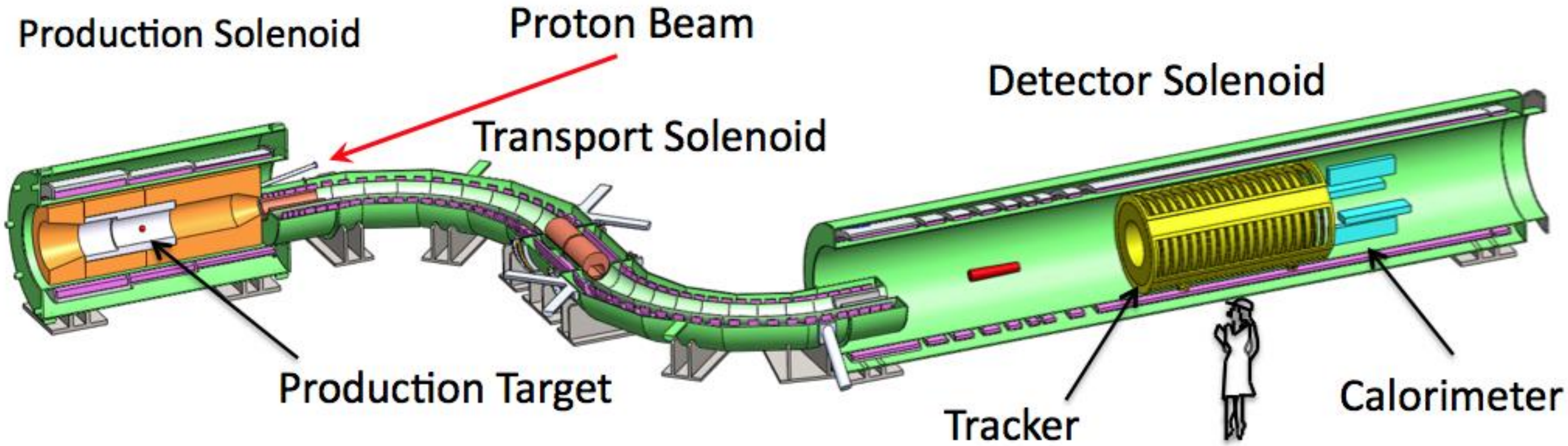


Cores from Google

CMS @ Google – preliminary numbers

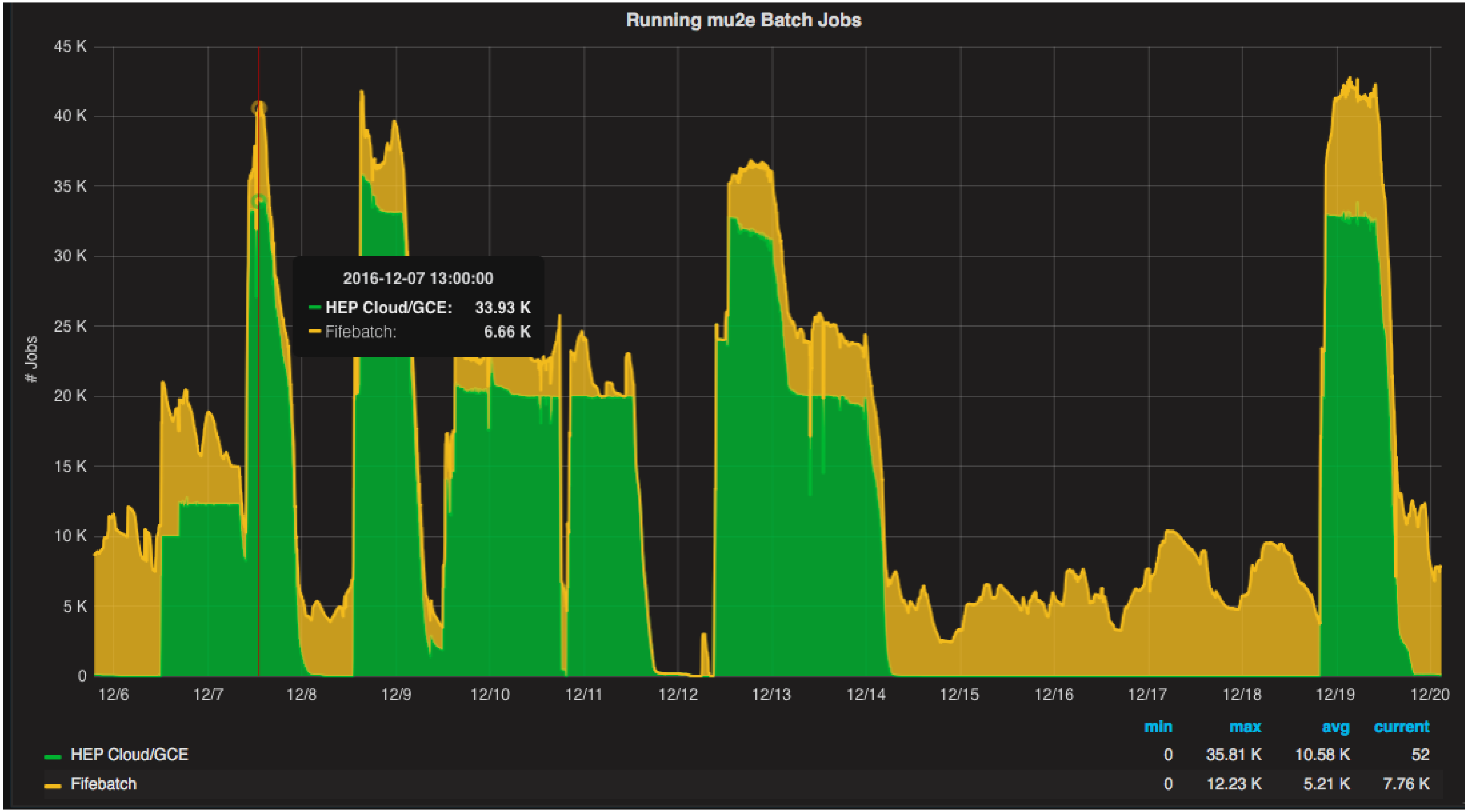
- 6.35 M wallhours used; 5.42 M wallhours for completed jobs.
  - 730172 simulation jobs submitted; only 47 did not complete through the CMS and HEPCloud fault-tolerant infrastructures
  - Most wasted hours during ramp-up as we found and eliminated issues; goodput was at 94% during the last 3 days.
- Used ~$100k worth of credits on Google Cloud during Supercomputing 2016
  - $71k virtual machine costs
  - $8.6k network egress
  - $8.5k disk attached to VMs
  - $3.5k cloud storage for input data
- 205 M physics events generated, yielding 81.8 TB of data

Mu2e experiment



- Charged Lepton Flavor Violation is a near-universal feature of extensions to the Standard Model of particle physics
- Rare muon processes offer the best combination of new physics reach and experimental sensitivity
- **Search for muon (in bound state) converting to an electron (“mu” to “e”)**

Mu2e – executing on Google Cloud



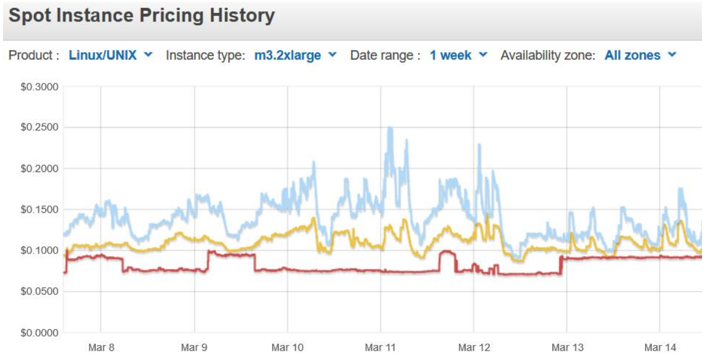
	min	max	avg	current
🟩 HEP Cloud/GCE	0	35.81 K	10.58 K	52
🟨 Fifebatch	0	12.23 K	5.21 K	7.76 K

Commercial Cloud Pricing

- Significant costs on Commercial Cloud
  - Compute charges over time (per hour)*
  - Persistent storage for large input data sets
  - Ancillary support services (persistent scalable web caches)
  - Per-operation API charges

VM Pricing: using the AWS "Spot Market"

- AWS has a fixed price per hour (rates vary by machine type)
- Excess capacity is released to the free ("spot") market at a fraction of the on-demand price
  - End user chooses a bid price
  - If (market price < bid), you pay only market price for the provisioned resource
    - If (market price > bid), you don't get the resource
  - If the price fluctuates while you are running and the market price exceeds your original bid price, you may get kicked off the node (with a 2 minute warning!)



Spot Instance Pricing History

Product : Linux/UNIX Instance type: m3.2xlarge Date range : 1 week Availability zone: All zones

VM Pricing: using Google preemptible VMs

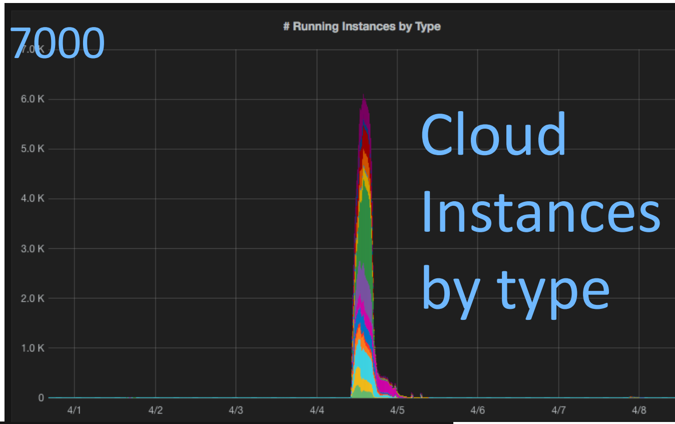
- Google VMs have a fixed cost (varies by machine types)
- Preemptible Google VMs are available at a significantly smaller fixed cost – 1 cent per core hour for a “standard candle”
  - We saved a few percent on cost by using custom VMs (2 GB per core instead of the standard 3.75 GB per core)

On-premises vs. cloud cost comparison - AWS

- Average cost per core-hour
  - On-premises resource: **.9** cents per core-hour
    - Includes power, cooling, staff
  - Off-premises at AWS: **1.4** cents per core-hour
    - Ranged up to 3 cents per core-hour at smaller scale
- Benchmarks
  - Specialized (“ttbar”) benchmark focused on HEP workflows
    - On-premises: **0.0163** (higher = better)
    - Off-premises: **0.0158**
- Raw compute performance roughly equivalent
- Cloud costs larger – but approaching equivalence
  - Still analyzing Google data; back-of-envelope ~ **1.6** cents per core-hour

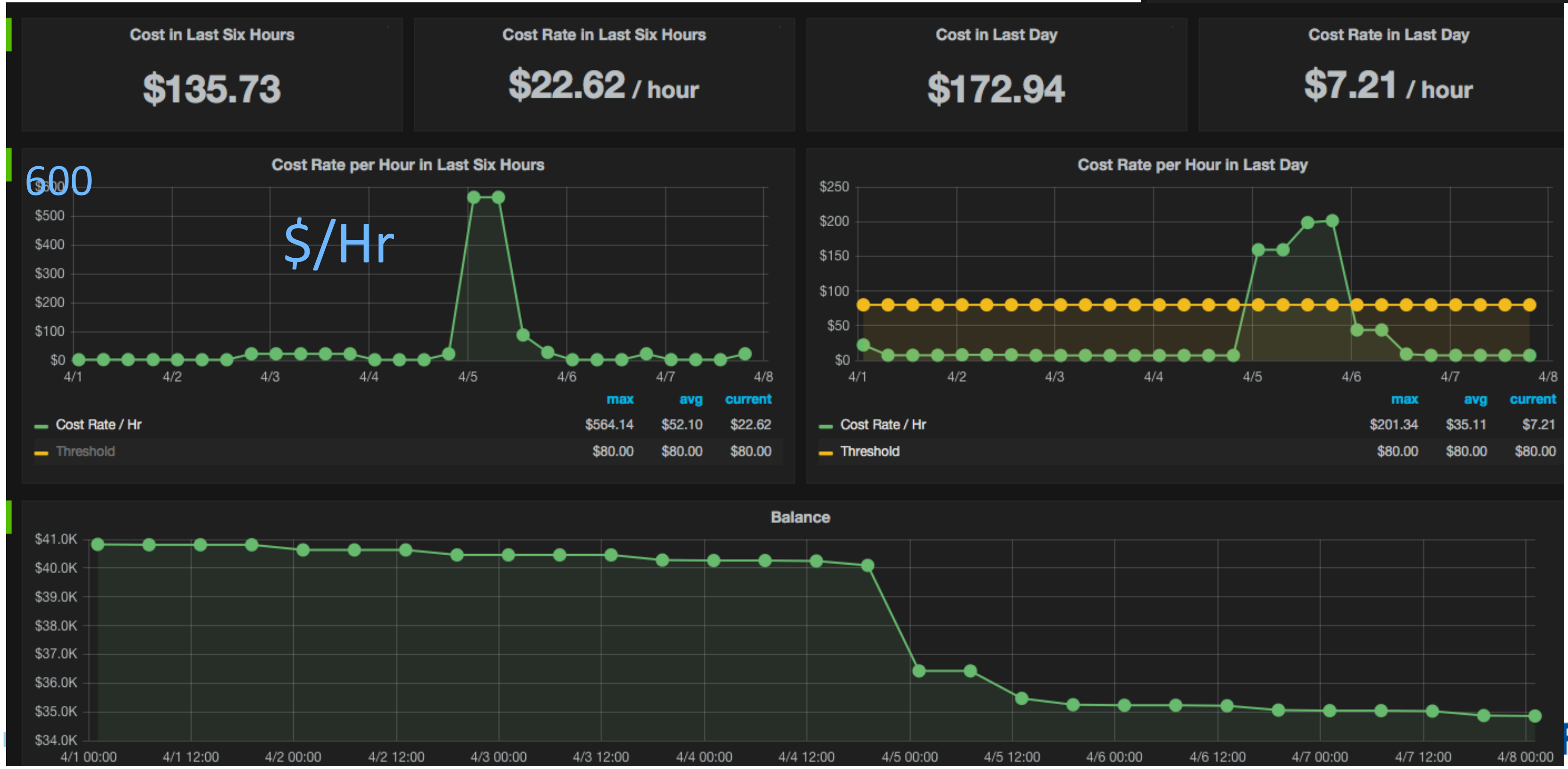
HEPCloud: Orchestration

- Monitoring and Accounting
  - Synergies with FIFE monitoring projects
    - But also monitoring real-time expense
  - Feedback loop into Decision Engine



7000

Cloud Instances by type



Cost in Last Six Hours
$135.73

Cost Rate in Last Six Hours
$22.62 / hour

Cost in Last Day
$172.94

Cost Rate in Last Day
$7.21 / hour

Cost Rate per Hour in Last Six Hours

	max	avg	current
Cost Rate / Hr	$564.14	$52.10	$22.62
Threshold	$80.00	$80.00	$80.00

Cost Rate per Hour in Last Day

	max	avg	current
Cost Rate / Hr	$201.34	$35.11	$7.21
Threshold	$80.00	$80.00	$80.00

Balance

600

$/Hr

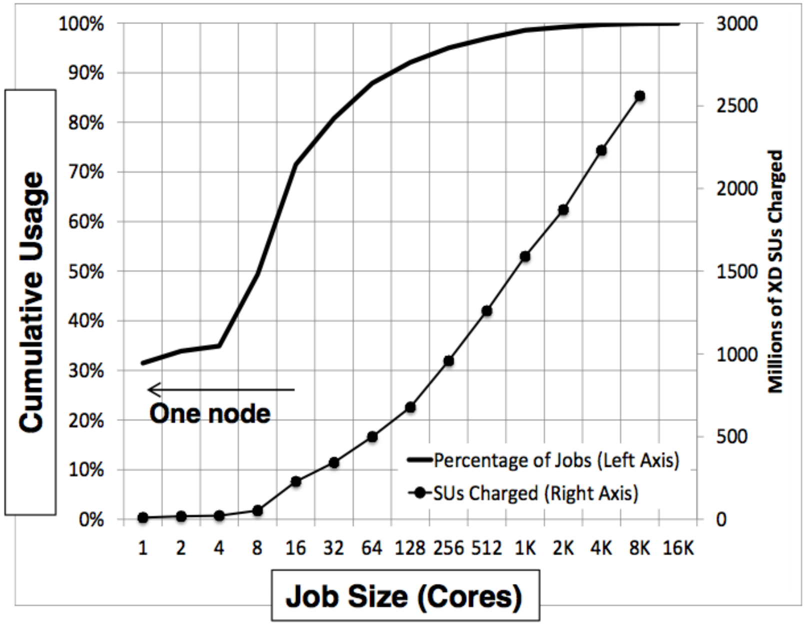
HEPCloud Compute and HPC

- A very appealing possibility, as we are approaching the exascale era, is to consider HPC facilities as a potential compute resource for HEPCloud
  - and, in the other direction, consider HEPCloud facility services (e.g. storage) as a potential resource for HPC facilities
- Investigate use cases with workflows that will allow such utilization within the constraints of allocation, security and access policy of HPC facilities.
- Initiate work with HPC facilities to fully understand constraints and requirements that will enable us to develop the HEPCloud process, policies and tools necessary for access of HPC resources

HPC: does it makes sense for our jobs?

HPC for the 99%

- **99% of jobs run on NSF's HPC resources in 2012 used <2,048 cores**
- **And consumed >50% of the total core-hours across NSF resources**



SDSC SAN DIEGO SUPERCOMPUTER CENTER

at the UNIVERSITY OF CALIFORNIA; SAN DIEGO

UCSD

From Michael Norman @ SDSC

HEPCloud Compute and HPC

- **Early steps**: adapt HTC workflows to HPC facilities
  - MicroBooNE production on Cori @ NERSC
    - Successfully downloaded the entire MicroBooNE release, including LArSoft and the art framework onto Cori, using Shifter from dockerhub.
    - Executed single node tests of MicroBooNE Monte Carlo production, reading from and writing to the global scratch file system through the container
  - Pythia on Mira @ ALCF: multi-parameter tuning of event generators using collider data
    - MPI + multi-threading to execute 32k instances of Pythia and the Rivet analysis suite
    - Spirit of code-sharing – leveraged CMS contributions to multi-thread Pythia
  - CMS production on Edison, Cori @ NERSC: Provisioned resources and executed a variety of different GEN-SIM-DIGI-RECO workflows

HEPCloud Compute and HPC

- Early steps: adapt HTC workflows to HPC facilities
  - MicroBooNE production on Cori @ NERSC
  - Pythia on Mira @ ALCF
  - CMS production on Edison, Cori @ NERSC
- **Plans for 2017:** HEPCloud provisioning @ NERSC
  - HEPCloud allocation granted for 28 million MPP-hours
    - 16 million MPP-hours for intensity frontier (mu2e, MicroBooNE, NOvA, …)
    - 12 million MPP-hours for CMS
      - CMS production will run Knight's Landing; experiment is working to optimize and maximize efficiency
  - Leverage experience

Thanks

- The Fermilab team:
  - Joe Boyd, Stu Fuess, Gabriele Garzoglio, Hyun Woo Kim, Rob Kennedy, Krista Majewski, David Mason, Parag Mhashilkar, Neha Sharma, Steve Timm, Anthony Tiradani, Panagiotis Spentzouris
- The HTCondor and glideinWMS projects
- Open Science Grid
- Energy Sciences Network
- The Google team:
  - Karan Bhatia, Solomon Boulos, Sam Greenfield, Paul Rossman, Doug Strain
- The AWS team:
  - Sanjay Padhi, Jamie Baker, Jamie Kinney, Mike Kokorowski
- Resellers: Onix, DLT

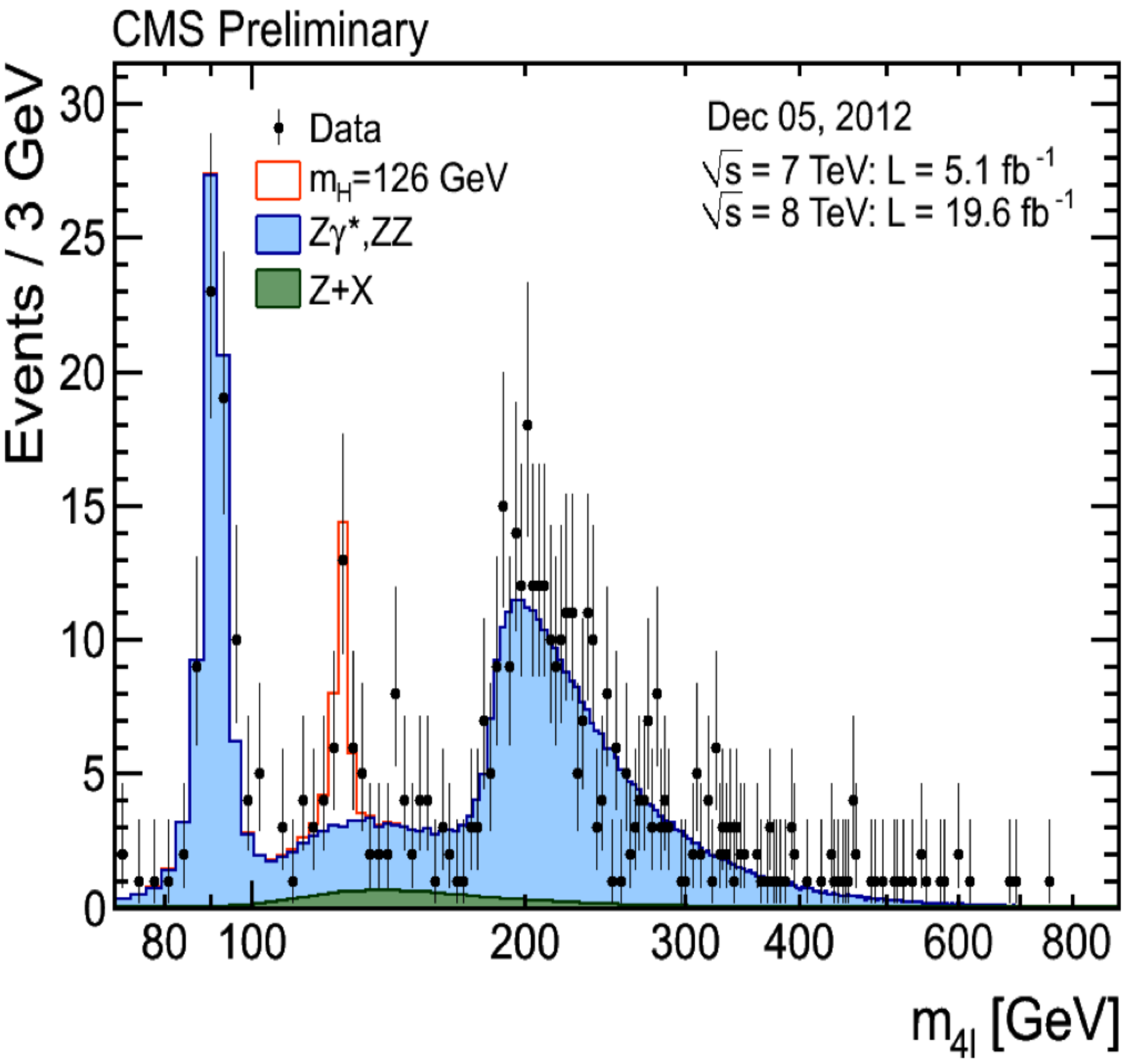
http://hepcloud.fnal.gov

Backup

Running on Google Cloud - Google Services

- Distributing experiment code (many versions and codes)
  - CVMFS: caching layer using squid web caches
  - Scalable, easy-to-manage software distribution
  - Good fit for **Google Load Balancing**
- Reading input data
  - Staged 500 TB of input data to **Google Cloud Storage**
    - Standard HEP and CMS data management tools now speak http!
    - **Thanks to ESNet and Google** for upgraded (100 Gbit+) peering!
  - Mounted data using **gcsfuse**
    - Good for big serial reads
- Monitoring
  - **Stackdriver logging**
    - Splunk-like functionality – a big help for troubleshooting

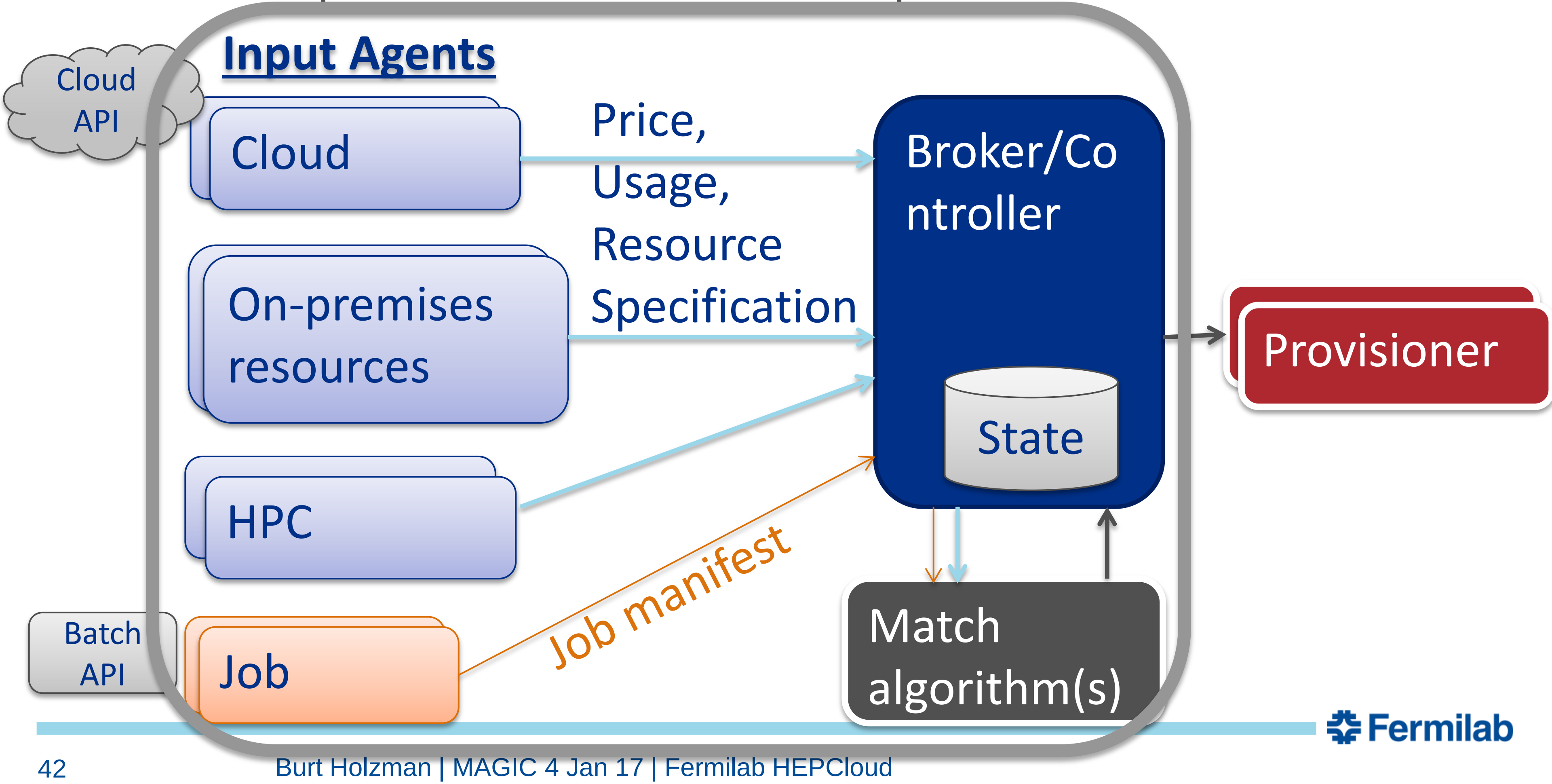
How is the science done?



- Particle Physics: **Statistical Science**
- Comparison with what we know (Standard Model)
- Analyze all data and look for deviations ➜ Needle in the Haystack

Decision Engine – design & architecture

- Decision Engine chooses what to provision next
  - v1.5 implementation: Strict matching based on processing type
  - v2.0 implementation: Zeroth-order prioritization based on cost



Pythia on Mira – Details

- We incorporated MPI into the main routines, using scatter and broadcast to send out unique parameters. The plan is to start one process on each node, running 64 threads, each with an instance of the pythia-based analysis. We will do this in chunk of 128 nodes, where each chunk is a gather collection point for writing to disk.

- Things were running on our x86 cluster - the porting to power PC of the build tools was the challenging part.

- ~150 core test

Description of CMS workflow

- Four chained steps (output of step N is input of step N+1)
  - Step 1 requires few GB input (“Gridpack”) – same files per job
  - Step 2 requires additional input: “pile-up” data (simulating multiple events per bunch crossing), 5-10 GB

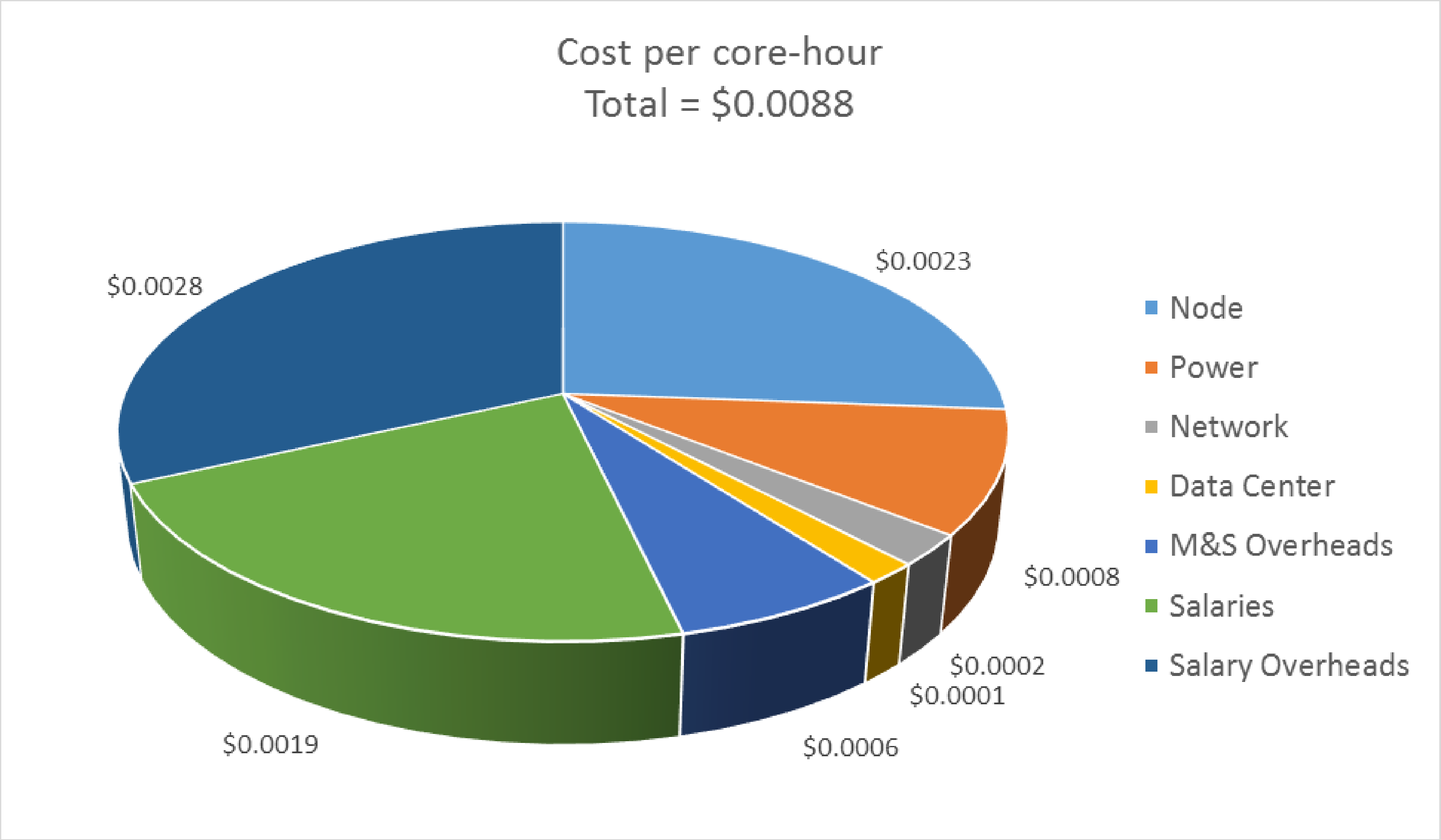
- Pile-up data is constructed on-the-fly by random seek and sequential reads into a 500 TB dataset
  - Staged pile-up datasets to Google Cloud Storage (storage service) ahead-of-time using FTS3 and PhEDEx – standard HEP grid tools and CMS data placement service

Reading pile-up from Google Cloud Storage

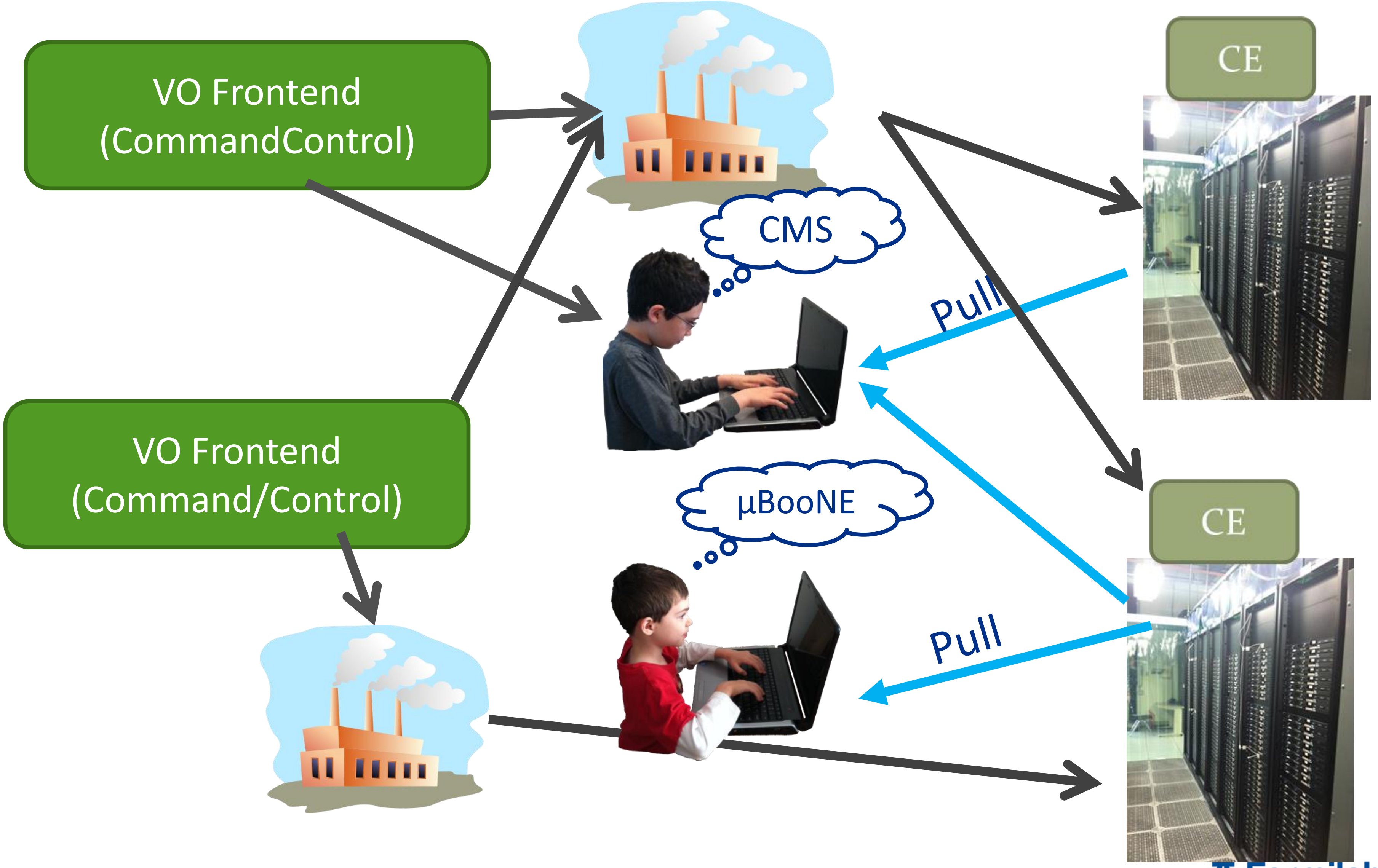
- Mounted regional bucket via gcsfuse on glide-in startup to /gcsfuse
- Used HTCondor “additional_json_file” functionality to specify role tied to image

Elements of the cost per core-hour

Based on Fermilab CMS Tier-1



glideinWMS – Building dynamic HTCondor pools



HEPCloud: Networking

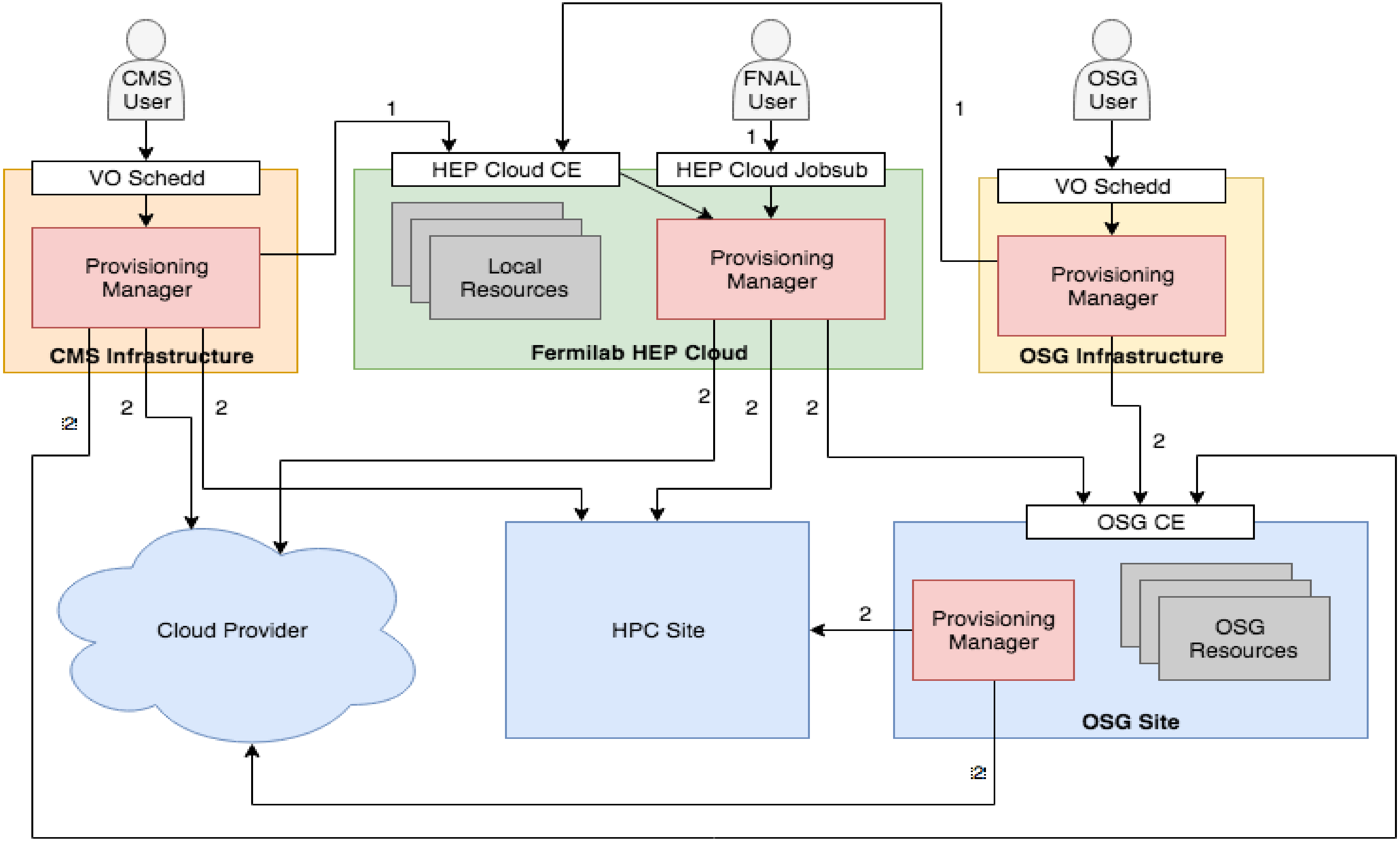
- All models of distributing computing rely on the performance of the underlying (local and wide-area) network
- Fermilab is approaching **1 Terabit** data center – connect to Energy Sciences Network (ESNet) at 4*100 Gigabit
  - ESNet enables distributed computing beyond ESNet sites: 100 Gigabit peering points with other networks

- Zone-based security protection of network resources
- On-demand (**Software Defined Network**-based) traffic controls
- Virtualization of network resources

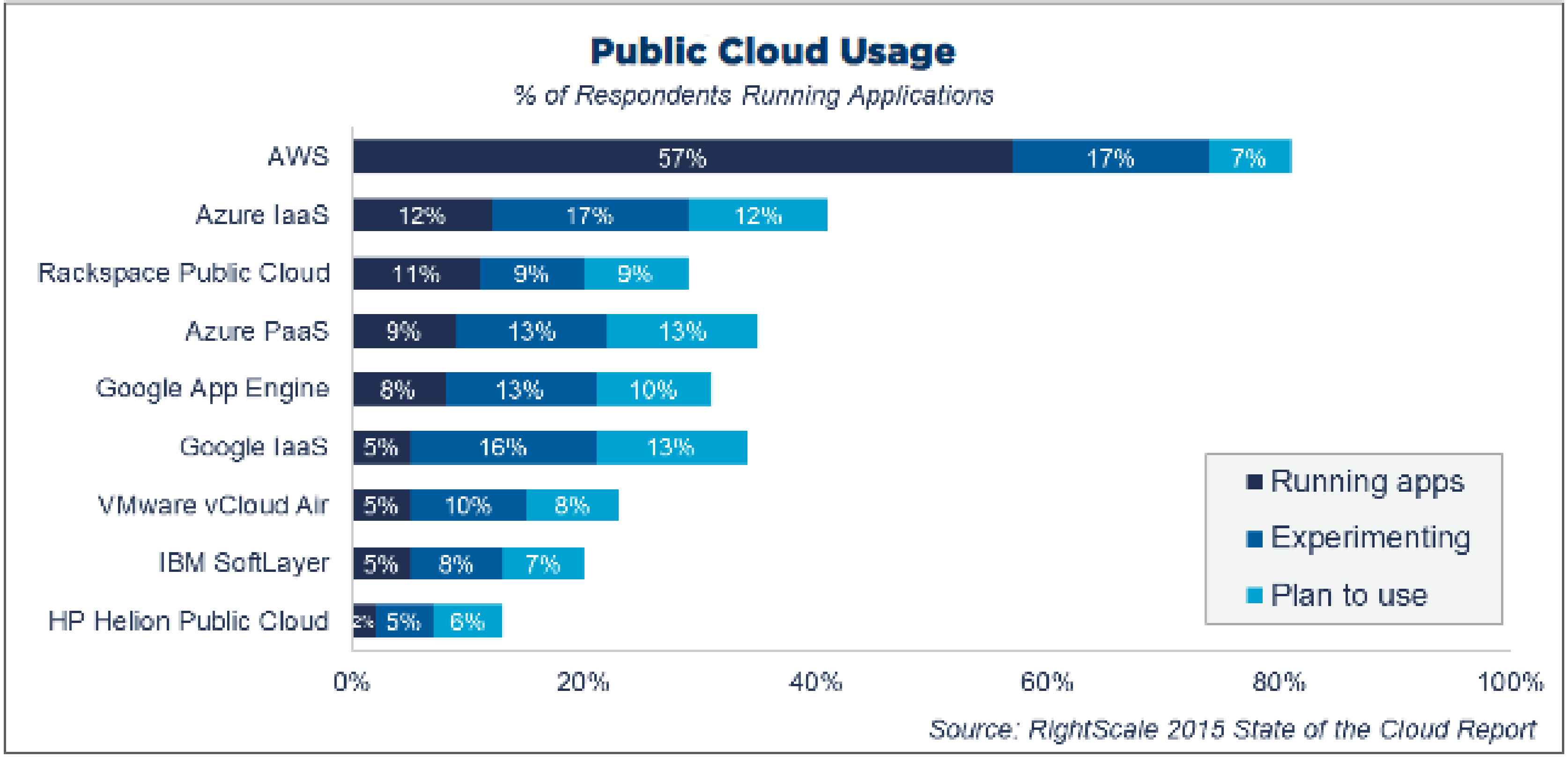
HEPCloud: Storage

- Data is the lifeblood of science
  - HEP experiments generate it by the station-wagon-load
  - Fermilab is a leader in the field in storing and serving petabytes of data to the world
- We are working with industry and other collaborators to modernize our services
  - Data storage and retrieval
  - Data cataloging
  - Support multiple-layer storage infrastructure approach
- One part of HEPCloud is to understand how to integrate all of these components – always driven by the experiment needs, both present and future

User’s View of HEPCloud



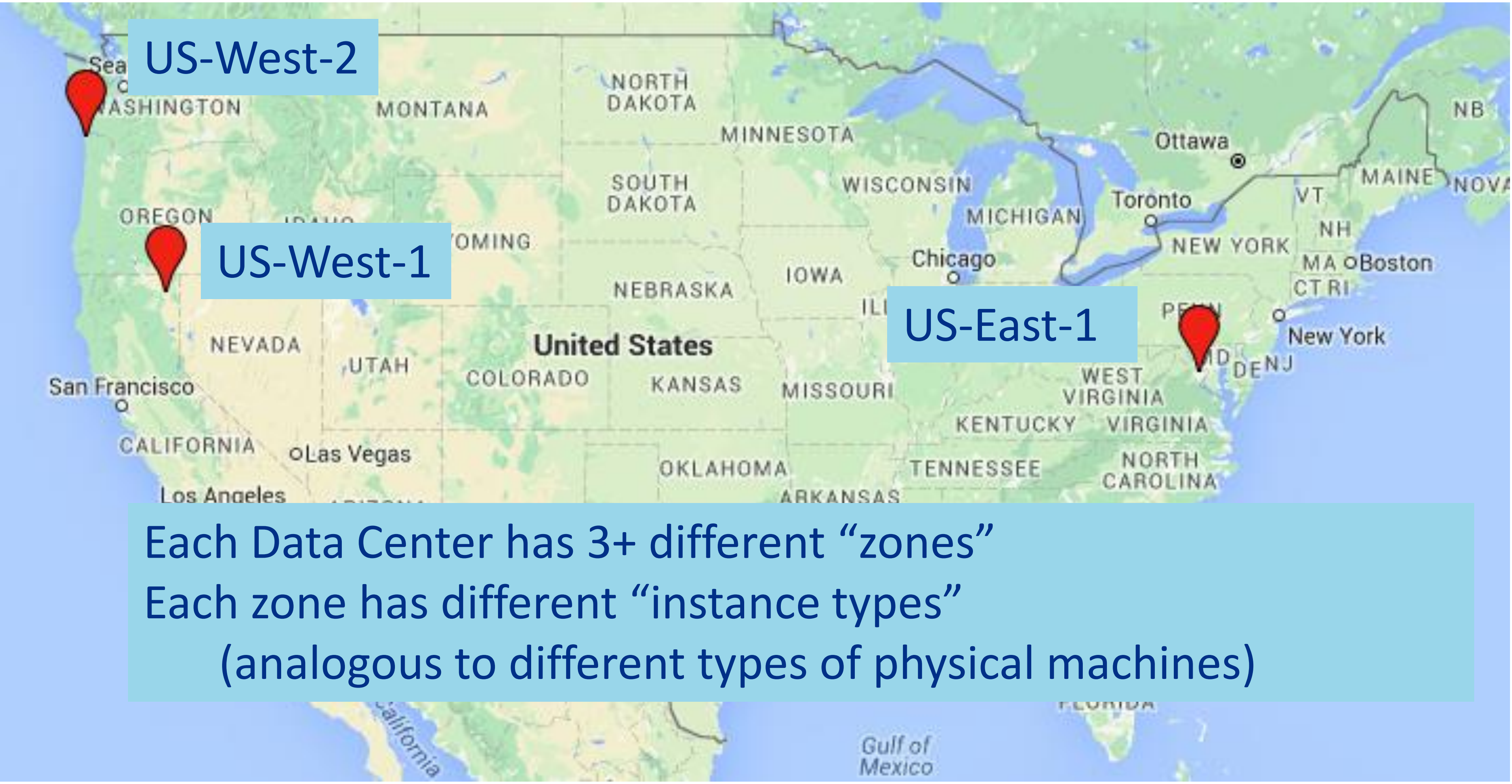
Fermilab HEPCloud: expanding to the Cloud



Source: RightScale 2015 State of the Cloud Report

Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof.

AWS topology – three US data centers (“regions”)



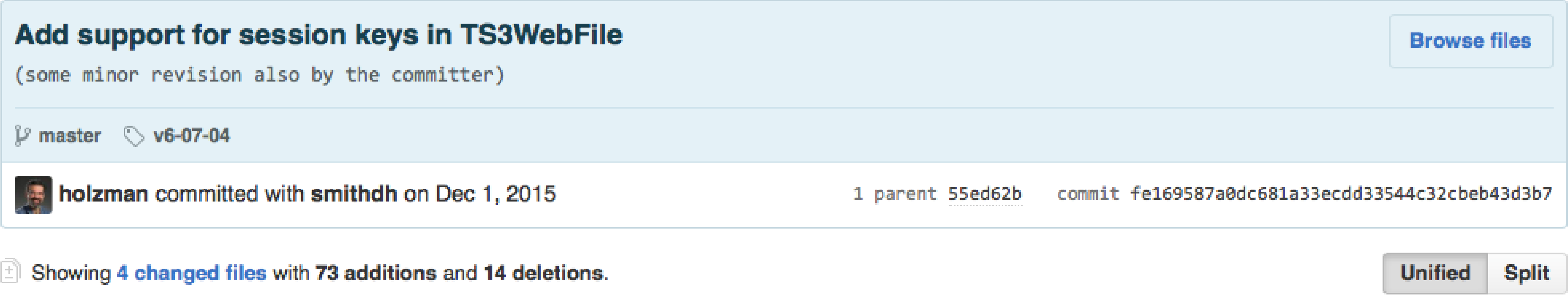
Each Data Center has 3+ different “zones”

Each zone has different “instance types”

(analogous to different types of physical machines)

Reading pile-up from AWS S3 (storage)

- AWS worker nodes granted permission to read from AWS S3 folder (“bucket”) via AWS Security-Token-Service (STS)
- ROOT has a TS3WebFile class!
  - But session key support was missing (needed for STS!)



Add support for session keys in TS3WebFile

```
(some minor revision also by the committer)
```

holzman committed with **smithdh** on Dec 1, 2015

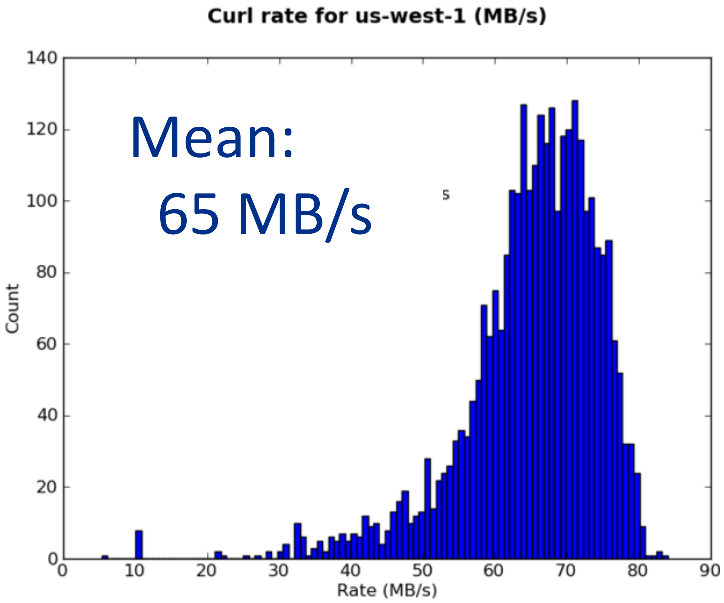
```
1 parent 55ed62b    commit fe169587a0dc681a33ecdd33544c32cbeb43d3b7
```

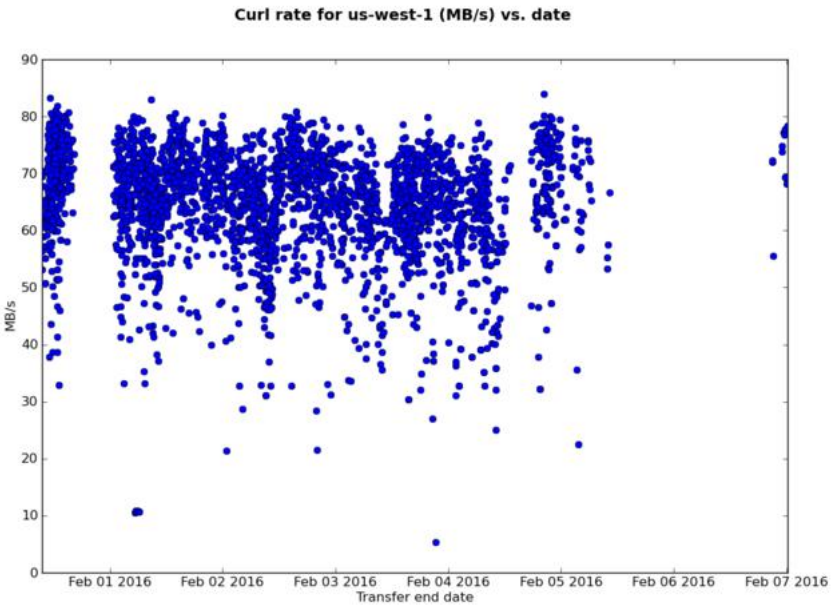
Showing 4 changed files with **73 additions** and **14 deletions**.

- This worked great!
  - Except…

Reading pile-up from AWS S3 (storage)

- Cost of data access was 30% of compute costs
  - 150 million HTTP GETs per hour is a lot!
- Wrote a curl wrapper to provide the custom AWS authentication headers
  - (Not often I can say I reduced costs by 5 orders of magnitude!)


Mean: 65 MB/s


Curl rate for us-west-1 (MB/s) vs. date
MB/s
Transfer end date
Feb 01 2016
Feb 02 2016
Feb 03 2016
Feb 04 2016
Feb 05 2016
Feb 06 2016
Feb 07 2016